

Chromic acetylacetonate

Other names:	(CH ₃ COCHCOCH ₃) ₃ Cr Chromium triacetylacetonate Chromium tris(2,4-pentanedionate) Chromium tris(acetylacetonate) Chromium(3+) acetylacetonate Chromium(3+), tris(2,4-pentanedionato)- Chromium(III) acetylacetonate Chromium(III) tris(2,4-pentanedionate) Chromium, tris(2,4-pentanedionato)- Chromium, tris(2,4-pentanedionato-O,O')- Chromium, tris(2,4-pentanedionato-O,O')-, (OC-6-11)- Chromium, tris(2,4-pentanedionato-«kappa»O,«kappa»O')-, (OC-6-11)- Chromium, tris(acetylacetonato)- NSC 4654 Tris(acetylacetonato)chromium Tris(acetylacetonato)chromium(III) chromium acetylacetonate chromium(III) 4-oxopent-2-ene-2-olate tris(2,4-pentanedionato)chromium
Inchi:	InChI=1S/3C5H8O2.Cr/c3*1-4(6)3-5(2)7;/h3*3,6H,1-2H3;/q;;;+3/p-3/b3*4-3-;
InchiKey:	JWORPXLMBPOPPU-LNTINUHCSA-K
Formula:	C ₁₅ H ₂₁ CrO ₆
SMILES:	CC(=O)C=C(C)[O-].CC(=O)C=C(C)[O-].CC(=O)C=C(C)[O-].[Cr]
Mol. weight [g/mol]:	349.32
CAS:	21679-31-2

Physical Properties

Property code	Value	Unit	Source
ea	0.87 ± 0.04	eV	NIST Webbook
hsub	126.80 ± 4.20	kJ/mol	NIST Webbook
hsub	132.10 ± 1.90	kJ/mol	NIST Webbook
hsub	123.00 ± 3.00	kJ/mol	NIST Webbook
hsub	110.90 ± 0.80	kJ/mol	NIST Webbook
ie	7.00 ± 0.20	eV	NIST Webbook
ie	7.87 ± 0.12	eV	NIST Webbook
ie	8.10 ± 0.05	eV	NIST Webbook
ie	7.50	eV	NIST Webbook

ie	7.46 ± 0.07	eV	NIST Webbook
tf	481.90 ± 0.50	K	NIST Webbook
tf	487.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	7.71	J/mol×K	10.37	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	11.29	J/mol×K	12.37	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	15.81	J/mol×K	14.67	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	20.74	J/mol×K	17.00	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	26.83	J/mol×K	19.75	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	32.26	J/mol×K	22.21	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	34.53	J/mol×K	23.22	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	37.47	J/mol×K	24.48	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	37.58	J/mol×K	24.55	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	40.95	J/mol×K	25.99	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	44.23	J/mol×K	27.39	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	45.34	J/mol×K	27.85	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	50.22	J/mol×K	29.83	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	52.01	J/mol×K	30.57	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	54.95	J/mol×K	31.91	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	60.06	J/mol×K	34.08	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	65.82	J/mol×K	36.42	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	68.09	J/mol×K	37.30	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	77.45	J/mol×K	41.15	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	81.84	J/mol×K	42.87	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	83.19	J/mol×K	43.47	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	89.53	J/mol×K	45.92	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	92.22	J/mol×K	46.92	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	98.41	J/mol×K	49.30	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	103.88	J/mol×K	51.32	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	108.90	J/mol×K	53.16	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	117.05	J/mol×K	55.97	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	120.29	J/mol×K	57.04	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	122.64	J/mol×K	58.09	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	128.56	J/mol×K	60.55	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	128.91	J/mol×K	60.56	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	136.27	J/mol×K	63.91	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	136.96	J/mol×K	64.15	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	139.62	J/mol×K	65.54	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	144.65	J/mol×K	67.85	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	150.92	J/mol×K	70.92	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	152.87	J/mol×K	71.78	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	161.57	J/mol×K	75.78	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	161.53	J/mol×K	75.84	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	164.11	J/mol×K	76.87	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	168.72	J/mol×K	79.05	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	170.69	J/mol×K	80.06	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	173.16	J/mol×K	81.28	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	175.06	J/mol×K	82.06	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	177.41	J/mol×K	83.26	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	179.57	J/mol×K	84.38	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	180.83	J/mol×K	84.96	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	184.81	J/mol×K	86.91	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	186.77	J/mol×K	87.94	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	187.58	J/mol×K	88.47	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	192.12	J/mol×K	90.71	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	193.56	J/mol×K	91.61	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	200.01	J/mol×K	94.95	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	201.14	J/mol×K	95.50	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	207.84	J/mol×K	99.24	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	207.72	J/mol×K	99.28	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	214.82	J/mol×K	103.58	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	220.43	J/mol×K	106.80	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	225.53	J/mol×K	110.04	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	232.64	J/mol×K	114.71	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	239.53	J/mol×K	119.52	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	246.37	J/mol×K	124.45	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	253.52	J/mol×K	129.50	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	260.04	J/mol×K	134.54	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	266.03	J/mol×K	139.45	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	272.10	J/mol×K	144.36	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	448.89	J/mol×K	317.49	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	284.09	J/mol×K	154.65	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	289.93	J/mol×K	159.87	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	295.59	J/mol×K	165.11	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	301.31	J/mol×K	170.26	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	305.92	J/mol×K	174.76	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	310.45	J/mol×K	179.21	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	315.44	J/mol×K	184.02	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	320.27	J/mol×K	188.75	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	325.12	J/mol×K	193.51	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	329.94	J/mol×K	198.29	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	335.55	J/mol×K	203.71	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	340.75	J/mol×K	209.36	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	346.27	J/mol×K	214.53	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	351.86	J/mol×K	219.64	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	356.22	J/mol×K	224.51	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	361.44	J/mol×K	229.67	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	366.76	J/mol×K	235.31	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	372.10	J/mol×K	240.88	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	377.18	J/mol×K	246.38	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	382.68	J/mol×K	251.83	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	388.87	J/mol×K	257.71	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	394.88	J/mol×K	263.50	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	400.54	J/mol×K	268.77	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	407.45	J/mol×K	275.50	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	409.89	J/mol×K	277.87	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	413.33	J/mol×K	281.32	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature

cps	417.22	J/mol×K	285.19	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	421.14	J/mol×K	288.93	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	424.92	J/mol×K	292.64	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	428.72	J/mol×K	296.43	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	432.75	J/mol×K	300.42	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	436.63	J/mol×K	304.53	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	440.79	J/mol×K	308.77	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	444.86	J/mol×K	313.07	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	278.01	J/mol×K	149.43	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
cps	453.39	J/mol×K	321.88	Heat capacity and Raman spectra of Cr(C ₅ H ₇ O ₂) ₃ at low temperature
hfust	34.00	kJ/mol	481.90	NIST Webbook
hfust	35.90	kJ/mol	486.00	NIST Webbook
hfust	34.00	kJ/mol	489.00	NIST Webbook
hfust	28.70	kJ/mol	487.00	NIST Webbook
hfust	35.20	kJ/mol	490.00	NIST Webbook
hfust	28.40	kJ/mol	489.00	NIST Webbook
hsubt	128.20	kJ/mol	377.50	NIST Webbook
hsubt	127.60	kJ/mol	354.00	NIST Webbook

hsubt	111.60	kJ/mol	396.00	NIST Webbook
hsubt	91.00	kJ/mol	428.00	NIST Webbook
hsubt	113.00 ± 4.80	kJ/mol	471.50	NIST Webbook
hsubt	28.90	kJ/mol	463.00	NIST Webbook
hsubt	40.20 ± 1.70	kJ/mol	378.00	NIST Webbook
hsubt	112.10	kJ/mol	390.00	NIST Webbook
hvapt	120.80	kJ/mol	486.10	Determination of the enthalpies of sublimation and evaporation from thermogravimetric data: Application to metalorganic complexes of Al and Cr
hvapt	82.20 ± 2.00	kJ/mol	513.00	NIST Webbook
psub	1.68e-07	kPa	320.15	Thermodynamics of chromium acetylacetonate sublimation
psub	5.07e-07	kPa	327.15	Thermodynamics of chromium acetylacetonate sublimation
psub	7.54e-07	kPa	330.00	Thermodynamics of chromium acetylacetonate sublimation
psub	1.27e-06	kPa	333.15	Thermodynamics of chromium acetylacetonate sublimation
psub	3.33e-06	kPa	341.15	Thermodynamics of chromium acetylacetonate sublimation
psub	8.40e-06	kPa	348.15	Thermodynamics of chromium acetylacetonate sublimation
psub	7.63e-04	kPa	388.15	Thermodynamics of chromium acetylacetonate sublimation
psub	4.60e-05	kPa	362.15	Thermodynamics of chromium acetylacetonate sublimation
psub	1.10e-04	kPa	369.15	Thermodynamics of chromium acetylacetonate sublimation
psub	2.25e-04	kPa	376.15	Thermodynamics of chromium acetylacetonate sublimation

psub	3.42e-04	kPa	380.00	Thermodynamics of chromium acetylacetonate sublimation
psub	4.40e-04	kPa	382.15	Thermodynamics of chromium acetylacetonate sublimation
psub	2.05e-05	kPa	355.15	Thermodynamics of chromium acetylacetonate sublimation
sfust	69.50	J/molxK	481.90	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C21679312&Units=SI>

Solubilities of cobalt(III) and chromium(III) acetylacetonates in chloroform and correlation of the diffusion coefficients of chromium(III) acetylacetonate in chloroform with thermodynamic data of chromium(III) acetylacetonate sublimation and in heat capacity and Raman spectra of Cr(C₅H₇O₂)₃ at low temperature: Determination of the enthalpies of sublimation and evaporation from thermogravimetric data: Application to metalorganic complexes of Al and Cr:

<https://www.doi.org/10.1016/j.fluid.2013.02.004>

Measurement and correlation of the diffusion coefficients of chromium(III) acetylacetonate in chloroform with thermodynamic data of chromium(III) acetylacetonate sublimation and in heat capacity and Raman spectra of Cr(C₅H₇O₂)₃ at low temperature:

<https://www.doi.org/10.1016/j.jct.2016.10.012>

Determination of the enthalpies of sublimation and evaporation from thermogravimetric data: Application to metalorganic complexes of Al and Cr:

<https://www.doi.org/10.1016/j.tca.2005.02.034>

<https://www.doi.org/10.1016/j.tca.2005.12.024>

<https://www.doi.org/10.1016/j.tca.2008.12.032>

Legend

cps:	Solid phase heat capacity
ea:	Electron affinity
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
psub:	Sublimation pressure
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point

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