

# Cycloheptanol

<b>Other names:</b>	SUBEROL
<b>Inchi:</b>	InChI=1S/C7H14O/c8-7-5-3-1-2-4-6-7/h7-8H,1-6H2
<b>InchiKey:</b>	QCRFMSUKWRQZEM-UHFFFAOYSA-N
<b>Formula:</b>	C7H14O
<b>SMILES:</b>	OC1CCCCC1
<b>Mol. weight [g/mol]:</b>	114.19
<b>CAS:</b>	502-41-0

## Physical Properties

Property code	Value	Unit	Source
chl	-4362.00 ± 1.00	kJ/mol	NIST Webbook
chl	-4429.20	kJ/mol	NIST Webbook
gf	-116.41	kJ/mol	Joback Method
hf	-291.88	kJ/mol	Joback Method
hfus	7.71	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-0.88		Aqueous Solubility Prediction Method
log10ws	-0.88		Estimated Solubility Method
logp	1.701		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1040.20		NIST Webbook
rinpol	1028.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1566.00		NIST Webbook
sl	241.64	J/molxK	NIST Webbook
tb	458.20	K	NIST Webbook
tc	675.73	K	Joback Method
tf	233.33	K	Joback Method
tt	280.30 ± 0.02	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.33	J/mol×K	675.73	Joback Method
cpg	244.83	J/mol×K	508.92	Joback Method
cpg	258.94	J/mol×K	542.28	Joback Method
cpg	272.33	J/mol×K	575.64	Joback Method
cpg	285.01	J/mol×K	609.00	Joback Method
cpg	297.01	J/mol×K	642.37	Joback Method
cpg	230.00	J/mol×K	475.56	Joback Method
cpl	250.22	J/mol×K	298.15	NIST Webbook
cpl	244.30	J/mol×K	298.00	NIST Webbook
cps	204.00	J/mol×K	270.00	Heat capacities of selected cycloalcohols
cps	204.00	J/mol×K	270.00	Heat capacities of selected cycloalcohols
cps	205.20	J/mol×K	271.34	Heat capacities of selected cycloalcohols
cps	201.70	J/mol×K	268.00	Heat capacities of selected cycloalcohols
cps	201.80	J/mol×K	268.00	Heat capacities of selected cycloalcohols
cps	199.80	J/mol×K	266.00	Heat capacities of selected cycloalcohols
cps	199.80	J/mol×K	266.00	Heat capacities of selected cycloalcohols
cps	198.10	J/mol×K	264.00	Heat capacities of selected cycloalcohols
cps	198.00	J/mol×K	264.00	Heat capacities of selected cycloalcohols
cps	196.50	J/mol×K	262.00	Heat capacities of selected cycloalcohols
cps	196.40	J/mol×K	262.00	Heat capacities of selected cycloalcohols
cps	195.40	J/mol×K	260.73	Heat capacities of selected cycloalcohols

cps	195.30	J/molxK	260.59	Heat capacities of selected cycloalcohols
cps	205.40	J/molxK	271.43	Heat capacities of selected cycloalcohols
dvisc	0.0183260	Paxs	273.70	Joback Method
dvisc	0.0044230	Paxs	314.07	Joback Method
dvisc	0.0014757	Paxs	354.44	Joback Method
dvisc	0.1241815	Paxs	233.33	Joback Method
dvisc	0.0006163	Paxs	394.82	Joback Method
dvisc	0.0001677	Paxs	475.56	Joback Method
dvisc	0.0003026	Paxs	435.19	Joback Method
hfust	1.51	kJ/mol	278.30	NIST Webbook
hfust	0.88	kJ/mol	258.40	NIST Webbook
hfust	1.60	kJ/mol	280.30	NIST Webbook
hfust	2.93	kJ/mol	172.20	NIST Webbook
hfust	1.60	kJ/mol	280.30	NIST Webbook
hfust	0.55	kJ/mol	227.30	NIST Webbook
hvapt	67.40	kJ/mol	302.50	NIST Webbook
hvapt	64.70	kJ/mol	303.50	NIST Webbook
pvap	0.01	kPa	288.22	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.02	kPa	293.72	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.02	kPa	293.73	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	7.50e-03	kPa	284.67	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.03	kPa	298.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.03	kPa	298.28	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	7.10e-03	kPa	284.35	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.04	kPa	303.37	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.06	kPa	307.00	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.07	kPa	308.15	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.08	kPa	310.11	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.12	kPa	315.14	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.16	kPa	319.51	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.18	kPa	320.88	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.02	kPa	292.50	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.03	kPa	298.44	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.02	kPa	293.86	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
sfust	3.39	J/molxK	258.40	NIST Webbook
sfust	16.98	J/molxK	172.20	NIST Webbook
sfust	5.72	J/molxK	280.30	NIST Webbook
sfust	2.44	J/molxK	227.30	NIST Webbook
srf	0.03	N/m	313.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.02	N/m	323.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol

srf	0.03	N/m	308.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	303.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	298.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	293.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol
srf	0.03	N/m	318.15	Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-2.66915e+01
Coeff. B	-5.85520e+03
Coeff. C	7.60167e+00
Coeff. D	-6.45886e-06
Temperature range (K), min.	284.15
Temperature range (K), max.	323.15

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol:** <https://www.doi.org/10.1021/je050055m>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**KDB Vapor Pressure Data:** <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=900>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

Vapor Pressure and Its Temperature  
Dependence of 28 Organic  
Compounds: Cyclic Amines, Cyclic  
Ethers, and Cyclic and Open Chain  
Secondary Alcohols:

<https://www.doi.org/10.1021/acs.jced.6b00576>

Heat capacities of selected  
cycloalcohols:  
Joback Method:

<https://www.thermo.com/files/research/kdb/mol/mol900.mol>

McGowan Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C502410&Units=SI>

<https://www.doi.org/10.1016/j.tca.2014.10.002>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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