Disulfide, dimethyl

Other names:	(CH3S)2
	(METHYLDITHIO)METHANE
	2,3-DITHIABUTANE
	DMDS
	Dimethyl disulfide
	Dimethyl disulphide
	Methyl disulfide
	Methyldisulfanylmethane
	NSC 9370
	Sulfa-Hitech
	UN 2381
	dimethyldisulfide
	disulfide, dimethyl-
Inchi:	InChI=1S/C2H6S2/c1-3-4-2/h1-2H3
InchiKey:	WQOXQRCZOLPYPM-UHFFFAOYSA-N
Formula:	C2H6S2
SMILES:	CSSC
Mol. weight [g/mol]:	94.20
CAS:	624-92-0

Physical Properties

Property code	Value	Unit	Source
af	0.2380		KDB
affp	815.30	kJ/mol	NIST Webbook
basg	782.80	kJ/mol	NIST Webbook
chl	-2786.50 ± 0.71	kJ/mol	NIST Webbook
ea	1.75	eV	NIST Webbook
ea	0.23 ± 0.21	eV	NIST Webbook
gf	32.20	kJ/mol	Joback Method
hf	-24.10 ± 0.84	kJ/mol	NIST Webbook
hf	-24.00	kJ/mol	NIST Webbook
hf	-24.10 ± 2.30	kJ/mol	NIST Webbook
hfl	-62.60 ± 2.00	kJ/mol	NIST Webbook
hfl	-62.47 ± 0.84	kJ/mol	NIST Webbook
hfpi	690.00 ± 15.00	kJ/mol	NIST Webbook
hfpiz	707.00 ± 15.00	kJ/mol	NIST Webbook
hfus	9.20	kJ/mol	Joback Method

hvap	33.68	kJ/mol	Joback Method
ie	8.33 ± 0.02	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.18 ± 0.03	eV	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	7.40 ± 0.30	eV	NIST Webbook
ie	8.20 ± 0.20	eV	NIST Webbook
ie	7.40 ± 0.10	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.46 ± 0.03	eV	NIST Webbook
ie	8.71 ± 0.03	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
log10ws	-1.44		Estimated Solubility Method
log10ws	-1.44		Aqueous Solubility Prediction Method
logp	1.627		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	5070.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
pc	4800.00	kPa	KDB
rinpol	765.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	736.00		NIST Webbook
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ripol	1094.00		NIST Webbook
sl	235.39	J/mol×K	NIST Webbook
tb	382.90	K	NIST Webbook
tb	382.90	K	KDB
tb	0.00	K	NIST Webbook
tb	383.00 ± 1.50	K	NIST Webbook
tb	381.15 ± 1.50	K	NIST Webbook
tb	382.90	K	NIST Webbook
tc	605.70	K	NIST Webbook
tc	615.00 ± 50.00	K	NIST Webbook
tc	605.00	K	KDB
tf	188.00	K	KDB

tf	188.50 ± 0.20	K	NIST Webbook
tt	188.44 ± 0.02	K	NIST Webbook
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.28	J/mol×K	494.40	Joback Method
cpg	118.73	J/mol×K	457.17	Joback Method
cpg	112.99	J/mol×K	419.95	Joback Method
cpg	139.78	J/mol×K	606.07	Joback Method
cpg	134.82	J/mol×K	568.85	Joback Method
cpg	129.65	J/mol×K	531.62	Joback Method
cpg	107.10	J/mol×K	382.72	Joback Method
cpl	146.11	J/mol×K	298.15	NIST Webbook
hfust	9.19	kJ/mol	188.40	NIST Webbook
hfust	9.19	kJ/mol	188.40	NIST Webbook
hfust	9.19	kJ/mol	188.44	NIST Webbook
hvapt	38.20	kJ/mol	310.50	NIST Webbook
hvapt	37.80	kJ/mol	349.50	NIST Webbook
hvapt	36.00 ± 0.10	kJ/mol	341.00	NIST Webbook
hvapt	34.90 ± 0.10	kJ/mol	360.00	NIST Webbook
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hvapt	36.70	kJ/mol	354.50	NIST Webbook
hvapt	33.78	kJ/mol	382.90	NIST Webbook
hvapt	33.68	kJ/mol	382.90	KDB
pvap	61.90	kPa	366.46	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	100.60	kPa	382.02	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K

pvap	90.90	kPa	378.75	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	81.10	kPa	375.04	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	72.90	kPa	371.63	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	53.90	kPa	362.18	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	41.70	kPa	354.42	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	31.10	kPa	346.26	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	18.20	kPa	332.19	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K

rfi	1.52260		298.00	Vapor-Liquid Equilibrium for Dimethyl Disulfide + Butane, + trans-But-2-ene, + 2-Methylpropane, + 2-Methylpropene, + Ethanol, and 2-Ethoxy-2-methylpropane
rhol	1051.14	kg/m3	303.15	Isobaric Vapor Liquid Equilibrium for the Binary Systems Dimethyl Disulfide + C1 C4 n-Alkanol at 40.000 and 101.325 kPa
sfust	48.78	J/mol×K	188.44	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46948e+01
Coeff. B	-3.46015e+03
Coeff. C	-3.95090e+01
Temperature range (K), min.	279.68
Temperature range (K), max.	615.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.00528e+01
Coeff. B	-7.14948e+03
Coeff. C	-9.71673e+00
Coeff. D	7.02902e-06
Temperature range (K), min.	188.44
Temperature range (K), max.	606.00

Sources

Liquid-Liquid Equilibria on Three Binary Systems: Methyl Cyclopropanecarboxalate + Water, Dimethyl Sulfide + Water, and Dimethyl Disulfide + Water:	https://www.doi.org/10.1021/je050326t
Vapor-Liquid Equilibrium for Dimethyl Sulfide + Butane, trans-But-2-ene + 2-Methylpropene, + 2-Ethoxy-2-methylpropane:	https://www.doi.org/10.1021/je200039y
Combined effects of polarity and temperature on the solubility of organic compounds:	https://www.doi.org/10.1016/j.jct.2011.11.020
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624920&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Isobaric Vapor Liquid Equilibrium for the Binary Systems Dimethyl Disulfide + C3-C4 n-Alkanol at 40.000 and 101.325 kPa:	https://www.doi.org/10.1021/acs.jced.7b00078
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1851.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1851
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence-Time Flow Method:	https://www.doi.org/10.1021/je060269j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K:	https://www.doi.org/10.1016/j.fluid.2010.02.043

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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