Dimethyl sulfide

Other names:	(CH3)2S
	2-Thiapropane
	2-Thiopropane
	DMS
	Dimethyl monosulfide
	Dimethyl sulphide
	Dimethyl thioether
	Dimethylsulfid
	Exact-S
	Methane, 1,1'-thiobis-
	Methane, thiobis-
	Methyl monosulfide
	Methyl sulfide
	Methyl sulphide
	Methyl thioether
	Methylthiomethane
	Sulfide, methyl-
	Sulfure de methyle
	Thiobismethane
	UN 1164
Inchi:	InChI=1S/C2H6S/c1-3-2/h1-2H3
InchiKey:	QMMFVYPAHWMCMS-UHFFFAOYSA-N
Formula:	C2H6S
SMILES:	CSC
Mol. weight [g/mol]:	62.13
CAS:	75-18-3

Physical Properties

Property code	Value	Unit	Source
af	0.1910		KDB
affp	830.90	kJ/mol	NIST Webbook
basg	801.20	kJ/mol	NIST Webbook
chl	-2181.50 ± 0.30	kJ/mol	NIST Webbook
dm	1.50	debye	KDB
gf	6.95	kJ/mol	KDB
hf	-32.40	kJ/mol	NIST Webbook
hf	-37.50 ± 2.00	kJ/mol	NIST Webbook

hf	-37.60 ± 0.59	kJ/mol	NIST Webbook
hf	-37.56	kJ/mol	KDB
hfl	-65.40 ± 1.50	kJ/mol	NIST Webbook
hfl	-60.20	kJ/mol	NIST Webbook
hfl	-65.44 ± 0.59	kJ/mol	NIST Webbook
hfus	5.07	kJ/mol	Joback Method
hvap	27.80	kJ/mol	NIST Webbook
hvap	27.80 ± 0.04	kJ/mol	NIST Webbook
hvap	27.50	kJ/mol	NIST Webbook
hvap	27.90	kJ/mol	NIST Webbook
hvap	27.90 ± 0.60	kJ/mol	NIST Webbook
hvap	27.90 ± 0.60	kJ/mol	NIST Webbook
hvap	27.99	kJ/mol	NIST Webbook
hvap	27.70	kJ/mol	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.71 ± 0.01	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.57 ± 0.04	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.68 ± 0.03	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.69 ± 0.02	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
log10ws	-0.45		Estimated Solubility Method
log10ws	-0.45		Aqueous Solubility Prediction Method
logp	0.979		Crippen Method
mcvol	55.390	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB

nfpah	%!d(float64=4)		KDB
pc	5530.00 ± 40.53	kPa	NIST Webbook
pc	5530.00	kPa	KDB
rhoc	300.73 ± 1.86	kg/m3	NIST Webbook
rhoc	308.93 ± 1.86	kg/m3	NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	503.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	503.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	529.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	505.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	516.00		NIST Webbook

rinpol	523.00	NIST Webbook
rinpol	523.00	NIST Webbook
rinpol	495.00	NIST Webbook
rinpol	506.00	NIST Webbook
rinpol	505.00	NIST Webbook
rinpol	505.00	NIST Webbook
rinpol	518.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	513.00	NIST Webbook
rinpol	521.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	511.00	NIST Webbook
rinpol	509.00	NIST Webbook
rinpol	500.00	NIST Webbook
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rinpol	513.00	NIST Webbook
rinpol	505.00	NIST Webbook
rinpol	500.00	NIST Webbook
rinpol	526.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	528.00	NIST Webbook
rinpol	523.00	NIST Webbook
rinpol	516.00	NIST Webbook
rinpol	515.00	NIST Webbook
rinpol	516.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	533.70	NIST Webbook
rinpol	543.60	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	530.20	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	508.00	NIST Webbook
rinpol	523.00	NIST Webbook
rinpol	522.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	500.00	NIST Webbook
rinpol	497.00	NIST Webbook
rinpol	500.00	NIST Webbook
rinpol	515.00	NIST Webbook

ripol	774.00	NIST Webbook
ripol	720.00	NIST Webbook
ripol	777.00	NIST Webbook
ripol	774.00	NIST Webbook
ripol	748.00	NIST Webbook
ripol	753.00	NIST Webbook
ripol	755.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	716.00	NIST Webbook
ripol	793.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	740.00	NIST Webbook
ripol	753.00	NIST Webbook
ripol	740.00	NIST Webbook
ripol	746.00	NIST Webbook
ripol	716.00	NIST Webbook
ripol	748.00	NIST Webbook
ripol	745.00	NIST Webbook
ripol	754.00	NIST Webbook
ripol	746.00	NIST Webbook
ripol	748.00	NIST Webbook
ripol	753.00	NIST Webbook
ripol	772.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	755.00	NIST Webbook
ripol	755.00	NIST Webbook
ripol	733.00	NIST Webbook
ripol	773.00	NIST Webbook
ripol	773.00	NIST Webbook
ripol	751.00	NIST Webbook
ripol	737.00	NIST Webbook
ripol	763.00	NIST Webbook
ripol	715.00	NIST Webbook
ripol	745.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	754.00	NIST Webbook
ripol	757.00	NIST Webbook
ripol	725.00	NIST Webbook
ripol	729.00	NIST Webbook
ripol	720.00	NIST Webbook
ripol	716.00	NIST Webbook
ripol	760.00	NIST Webbook
ripol	760.00	NIST Webbook

ripol	769.00		NIST Webbook
ripol	777.00		NIST Webbook
ripol	777.00		NIST Webbook
ripol	751.00		NIST Webbook
tb	310.50 ± 0.30	K	NIST Webbook
tb	310.48	K	KDB
tb	310.50	K	NIST Webbook
tb	310.60 ± 0.30	K	NIST Webbook
tb	311.20 ± 2.00	K	NIST Webbook
tb	310.55 ± 0.30	K	NIST Webbook
tb	310.50 ± 0.50	K	NIST Webbook
tb	316.20 ± 0.60	K	NIST Webbook
tb	310.60 ± 0.50	K	NIST Webbook
tb	310.50	K	NIST Webbook
tc	503.00 ± 0.40	K	NIST Webbook
tc	503.00 ± 0.40	K	NIST Webbook
tc	503.00	K	NIST Webbook
tc	503.00	K	KDB
tf	178.82	K	Aqueous Solubility Prediction Method
tf	174.80	K	KDB
tf	174.88 ± 0.06	K	NIST Webbook
tf	174.90 ± 0.10	K	NIST Webbook
tt	174.85 ± 0.03	K	NIST Webbook
vc	0.201	m3/kmol	KDB
zc	0.2657760		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.88	J/mol×K	313.94	Joback Method
cpg	79.79	J/mol×K	345.86	Joback Method
cpg	84.58	J/mol×K	377.78	Joback Method
cpg	89.24	J/mol×K	409.70	Joback Method
cpg	93.77	J/mol×K	441.62	Joback Method
cpg	98.17	J/mol×K	473.55	Joback Method
cpg	102.43	J/mol×K	505.47	Joback Method
hfust	7.98	kJ/mol	174.90	NIST Webbook
hfust	7.98	kJ/mol	174.90	NIST Webbook
hvapt	27.00	kJ/mol	310.50	NIST Webbook

hvapt	26.95	kJ/mol	310.70	KDB
hvapt	28.90	kJ/mol	293.50	NIST Webbook
hvapt	27.70	kJ/mol	343.00	NIST Webbook
hvapt	26.60	kJ/mol	412.50	NIST Webbook
hvapt	26.70	kJ/mol	475.00	NIST Webbook
hvapt	28.80 ± 0.10	kJ/mol	276.00	NIST Webbook
hvapt	27.90 ± 0.10	kJ/mol	292.00	NIST Webbook
hvapt	27.00 ± 0.10	kJ/mol	310.00	NIST Webbook
hvapt	28.20	kJ/mol	302.50	NIST Webbook
hvapt	28.90	kJ/mol	272.00	NIST Webbook
hvapt	28.90	kJ/mol	310.00	NIST Webbook
pvap	8.00	kPa	252.89	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	8.00	kPa	253.06	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)

pvap	22.00	kPa	272.76	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)	
pvap	29.00	kPa	278.46	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)	
pvap	53.00	kPa	293.16	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)	

pvap	54.00	kPa	293.43	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	112.00	kPa	313.30	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	112.00	kPa	313.43	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	91.70	kPa	307.86	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide

pvap	107.70	kPa	312.58	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	106.20	kPa	312.59	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	107.40	kPa	312.60	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	126.00	kPa	317.32	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	126.00	kPa	317.35	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	53.20	kPa	293.94	Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons
pvap	108.80	kPa	312.86	Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons
rfi	1.43127		298.15	Vapor-liquid equilibrium measurements of dimethylsulfide, +ethanol, +dimethylether, +methylacetate with a static total pressure method
rhol	848.00	kg/m3	293.00	KDB

srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42778e+01
Coeff. B	-2.64997e+03
Coeff. C	-3.66590e+01
Temperature range (K), min.	226.08
Temperature range (K), max.	503.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.57712e+01
Coeff. B	-4.97113e+03
Coeff. C	-6.21581e+00
Coeff. D	5.43587e-06
Temperature range (K), min.	174.88
Temperature range (K), max.	503.04

Sources

Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2010.03.027
Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + carbon dioxide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or methylmercaptan or ethylmercaptan):	https://www.doi.org/10.1016/j.fluid.2007.07.013
Liquid Liquid Equilibria on Three Binary Systems: Methyl Cyclopentanoxyacetate + Water; Dimethyl Sulfide + Water and Dimethyl Sulfide + Methyl Mercaptan:	https://www.doi.org/10.1021/je050326t
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814
Measurement of Henry s Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1 = 0.50 Using a Gas Stripping Technique:	https://www.doi.org/10.1021/je050268b
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide:	https://www.doi.org/10.1016/j.fluid.2008.01.030
Measurement through a Gas Stripping Technique of Henry's Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1 = 0.25 and 0.35:	https://www.doi.org/10.1021/je800349p
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Limiting Separation Factors and Limiting Activity Coefficients for Hexanal, 2-Methylbutanal, 3-Methylbutanal, and Dimethylsulfide in Water at (68.2 to 99.0) deg C:	https://www.doi.org/10.1021/je060324o
Determination of Henry's Law Constants and Activity Coefficients at Infinite Dilution of Flavor Compounds in Water at 298 K with a Gas-Chromatographic Method:	https://www.doi.org/10.1021/je0495942
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75183&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814
Measurement and correlation for the solubility of dimethyl succinylsuccinate in (methanol + water) and (methanol + dimethyl succinate) binary solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2014.04.012
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Vapor-liquid equilibrium measurements of dimethylsulfide, +ethanol, +dimethylether, +methylacetate with a static total pressure method:	https://www.doi.org/10.1016/j.fluid.2013.06.044

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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