

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	-37.56	kJ/mol	KDB
hf	-37.50 ± 2.00	kJ/mol	NIST Webbook

hf	-32.40	kJ/mol	NIST Webbook
hf	-37.60 ± 0.59	kJ/mol	NIST Webbook
hfl	-65.44 ± 0.59	kJ/mol	NIST Webbook
hfl	-60.20	kJ/mol	NIST Webbook
hfl	-65.40 ± 1.50	kJ/mol	NIST Webbook
hfus	5.07	kJ/mol	Joback Method
hvap	27.70	kJ/mol	NIST Webbook
hvap	27.80 ± 0.04	kJ/mol	NIST Webbook
hvap	27.80	kJ/mol	NIST Webbook
hvap	27.99	kJ/mol	NIST Webbook
hvap	27.90 ± 0.60	kJ/mol	NIST Webbook
hvap	27.90 ± 0.60	kJ/mol	NIST Webbook
hvap	27.90	kJ/mol	NIST Webbook
hvap	27.50	kJ/mol	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.69 ± 0.02	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.71 ± 0.01	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.57 ± 0.04	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.68 ± 0.03	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
ie	8.67	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	kPa	KDB
pc	5530.00 ± 40.53	kPa	NIST Webbook
rhoc	308.93 ± 1.86	kg/m3	NIST Webbook
rhoc	300.73 ± 1.86	kg/m3	NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	505.00		NIST Webbook
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ripol	733.00	NIST Webbook
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ripol	737.00	NIST Webbook
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ripol	754.00	NIST Webbook

ripol	745.00		NIST Webbook
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ripol	757.00		NIST Webbook
ripol	760.00		NIST Webbook
tb	310.50	K	NIST Webbook
tb	310.50	K	NIST Webbook
tb	310.60 ± 0.30	K	NIST Webbook
tb	311.20 ± 2.00	K	NIST Webbook
tb	310.50 ± 0.30	K	NIST Webbook
tb	310.50 ± 0.50	K	NIST Webbook
tb	310.60 ± 0.50	K	NIST Webbook
tb	316.20 ± 0.60	K	NIST Webbook
tb	310.55 ± 0.30	K	NIST Webbook
tb	310.48	K	KDB
tc	503.00	K	KDB
tc	503.00	K	NIST Webbook
tc	503.00 ± 0.40	K	NIST Webbook
tc	503.00 ± 0.40	K	NIST Webbook
tf	174.90 ± 0.10	K	NIST Webbook
tf	174.80	K	KDB
tf	178.82	K	Aqueous Solubility Prediction Method
tf	174.88 ± 0.06	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	93.77	J/mol×K	441.62	Joback Method
cpg	98.17	J/mol×K	473.55	Joback Method
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	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	28.90	kJ/mol	272.00	NIST Webbook

hvapt	28.90	kJ/mol	310.00	NIST Webbook
hvapt	26.95	kJ/mol	310.70	KDB
hvapt	27.00	kJ/mol	310.50	NIST Webbook
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
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
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 ethylmethysulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethysulfide 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
rfi	1.43127		298.15	Vapor-liquid equilibrium measurements of dimethylsulfide, +ethanol, +dimethylether, +methylacetate with a static total pressure method

rhoI	848.00	kg/m3	293.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

[illegible]

<https://www.doi.org/10.1016/j.fluid.2013.06.044>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

<https://www.doi.org/10.1016/j.fluid.2007.07.013>

<https://www.doi.org/10.1021/je060324o>

<https://www.doi.org/10.1021/je050326t>

<https://www.doi.org/10.1021/je050268b>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814>

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<https://www.doi.org/10.1016/j.fluid.2014.04.012>

https://en.wikipedia.org/wiki/Joback_method

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Infinite dilution activity coefficient and vapour liquid equilibrium
 methanol-dimethyl sulphide
 equilibrium for butane and butenes
 Mersmann and Linnhoff: a Gas Stripping
 Technique of Henry's Law Constants
 and Infinite Dilution Activity
 Coefficients of Propyl Mercaptan, Buty
 Mercaptan, and Dimethyl Sulfide in
 Methyl diethanolamine (1) + Water (2)
 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:
 KDB Pure (Korean Thermophysical
 Properties Databank):

<https://www.doi.org/10.1016/j.fluid.2010.03.027>

<https://www.doi.org/10.1016/j.fluid.2008.01.030>

<https://www.doi.org/10.1021/je800349p>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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

<https://www.doi.org/10.1021/je0495942>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C75183&Units=SI>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1814>

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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