Diethyl sulfide

Other names:	(C2H5)2S
	1,1'-Thiobisethane
	3-Thiapentane
	Diethyl sulphide
	Diethyl thioether
	Diethylsulfid
	Ethane, 1,1'-thiobis-
	Ethyl monosulfide
	Ethyl sulfide
	Ethyl thioether
	Ethylthioethane
	NSC 75157
	Sulfodor
	Thioethyl ether
	UN 2375
Inchi:	InChI=1S/C4H10S/c1-3-5-4-2/h3-4H2,1-2H3
InchiKey:	LJSQFQKUNVCTIA-UHFFFAOYSA-N
Formula:	C4H10S
SMILES:	CCSCC
Mol. weight [g/mol]:	90.19
CAS:	352-93-2

Physical Properties

Property code	Value	Unit	Source
affp	856.70	kJ/mol	NIST Webbook
basg	827.00	kJ/mol	NIST Webbook
chl	-3486.10 ± 0.67	kJ/mol	NIST Webbook
chl	-3471.00	kJ/mol	NIST Webbook
gf	15.92	kJ/mol	Joback Method
hf	-82.72 ± 0.79	kJ/mol	NIST Webbook
hf	-83.50 ± 2.30	kJ/mol	NIST Webbook
hfl	-119.40 ± 0.84	kJ/mol	NIST Webbook
hfl	-119.30 ± 2.00	kJ/mol	NIST Webbook
hfus	10.25	kJ/mol	Joback Method
hvap	31.32	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.46	eV	NIST Webbook

ie	8.44	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	8.42 ± 0.01	eV	NIST Webbook
ie	8.42 ± 0.01	eV	NIST Webbook
ie	8.43 ± 0.01	eV	NIST Webbook
log10ws	-1.34		Estimated Solubility Method
log10ws	-1.34		Aqueous Solubility Prediction Method
logp	1.759		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	3960.00 ± 40.53	kPa	NIST Webbook
rhoc	284.18 ± 1.80	kg/m3	NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	698.00		NIST Webbook

rinpol	703.70		NIST Webbook
rinpol	717.90		NIST Webbook
rinpol	708.50		NIST Webbook
rinpol	700.40		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	704.00		NIST Webbook
ripol	895.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	895.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	927.00		NIST Webbook
ripol	904.00		NIST Webbook
sl	269.28	J/mol×K	NIST Webbook
tb	359.70	K	Joback Method
tc	557.00 ± 0.50	K	NIST Webbook
tc	557.00	K	NIST Webbook
tf	169.85 ± 0.60	K	NIST Webbook
tf	169.24 ± 0.10	K	NIST Webbook
tf	169.85 ± 0.40	K	NIST Webbook
tf	169.18	K	Aqueous Solubility Prediction Method
tt	169.21 ± 0.02	K	NIST Webbook
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.04	J/mol×K	550.75	Joback Method
cpg	143.93	J/mol×K	391.54	Joback Method
cpg	152.12	J/mol×K	423.38	Joback Method
cpg	160.03	J/mol×K	455.23	Joback Method
cpg	167.65	J/mol×K	487.07	Joback Method
cpg	174.99	J/mol×K	518.91	Joback Method
cpg	135.44	J/mol×K	359.70	Joback Method
cpl	171.42	J/mol×K	298.15	NIST Webbook
hfust	11.90	kJ/mol	169.20	NIST Webbook
hfust	11.92	kJ/mol	169.20	NIST Webbook
hfust	11.90	kJ/mol	169.21	NIST Webbook

hvapt	31.77	kJ/mol	365.30	NIST Webbook
hvapt	34.90	kJ/mol	327.00	NIST Webbook
hvapt	34.40	kJ/mol	357.00	NIST Webbook
hvapt	34.80	kJ/mol	340.00	NIST Webbook
hvapt	37.50	kJ/mol	297.00	NIST Webbook
hvapt	33.50	kJ/mol	364.00	NIST Webbook
pvap	15.00	kPa	312.58	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
pvap	15.20	kPa	312.58	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
pvap	15.10	kPa	312.59	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
pvap	18.50	kPa	317.46	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
pvap	18.80	kPa	317.62	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene

pvap	13.30	kPa	307.94	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
rfi	1.43998		298.15	Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Diethylsulfide, + 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol
rfi	1.44000		298.15	Vapor liquid equilibrium for binary system of diethyl sulfide + cyclohexane at 353.15 and 343.15 K and diethyl sulfide + 2-ethoxy-2-methylpropane at 343.15 and 333.15 K
rfi	1.44000		298.15	Vapor-Liquid Equilibrium for Binary System of 1-Propanethiol, Thiophene, and Diethyl Sulfide with Toluene at 90.03 kPa
rfi	1.44000		298.15	Vapor-Liquid Equilibrium for Binary System of Diethyl Sulfide + n-Hexane at (338.15 and 323.15) K and Diethyl Sulfide + 1-Hexene at (333.15 and 323.15) K
rfi	1.44000		298.15	Vapor-Liquid Equilibrium for Binary System of Diethyl Sulfide + n-Heptane and Diethyl Sulfide + 2,2,4-Trimethylpentane at (363.15 and 353.15) K
sfust	70.35	J/mol×K	169.21	NIST Webbook

tcondl	0.14	W/m×K	273.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.14	W/m×K	293.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.14	W/m×K	313.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.13	W/m×K	333.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45990e+01
Coeff. B	-3.28325e+03
Coeff. C	-3.60380e+01
Temperature range (K), min.	265.45
Temperature range (K), max.	389.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.58385e+01
Coeff. B	-6.29676e+03
Coeff. C	-7.56818e+00

Coeff. D	5.03613e-06
Temperature range (K), min.	169.20
Temperature range (K), max.	557.15

Sources

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=1825

Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Diethylsulfide, + 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol: https://www.doi.org/10.1021/je3013028

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethylenimine, Tetrahydrothiophene, and Tetramethylethylenediamine: https://www.doi.org/10.1021/je0498661

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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Phase equilibria on binary systems containing diethyl sulfide: https://www.doi.org/10.1016/j.fluid.2010.11.026

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1825

Vapor-Liquid Equilibrium for Binary System of Diethyl Sulfide + n-Heptane and Diethyl Sulfide + 2,2,4-Trimethylpentane at (363.15 and 353.15) K: https://www.doi.org/10.1021/je060351e

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C352932&Units=SI

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

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

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McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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Vapor-Liquid Equilibrium for Binary System of 1-Propanethiol, Thiophene, and Diethyl Sulfide with Toluene at 90.03 kPa: https://www.doi.org/10.1021/je060093l

Legend

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical 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
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume