Diethyl disulfide

Other names:	(C2H5S)2
	1-(Ethyldisulfanyl)ethane
	3,4-Dithiahexane
	Diethyl disulphide
	Diethyldisulfid
	Disulfide, diethyl
	Ethyl disulfide
	Ethyl disulphide
	Ethyldithioethane
	NSC 8839
	diethyldisulfide
Inchi:	InChI=1S/C4H10S2/c1-3-5-6-4-2/h3-4H2,1-2H3
InchiKey:	CETBSQOFQKLHHZ-UHFFFAOYSA-N
Formula:	C4H10S2
SMILES:	CCSSCC
Mol. weight [g/mol]:	122.25
CAS:	110-81-6

Physical Properties

Property code	Value	Unit	Source
chl	-4087.70 ± 0.79	kJ/mol	NIST Webbook
ea	1.90	eV	NIST Webbook
gf	49.04	kJ/mol	Joback Method
hf	-74.70 ± 1.00	kJ/mol	NIST Webbook
hf	-74.60 ± 3.50	kJ/mol	NIST Webbook
hfl	-120.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-120.10 ± 1.00	kJ/mol	NIST Webbook
hfus	14.38	kJ/mol	Joback Method
hvap	38.13	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.27 ± 0.03	eV	NIST Webbook
ie	8.30 ± 0.15	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	-2.42		Estimated Solubility Method

log10ws	-2.42		Aqueous Solubility Prediction Method
logp	2.408		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	932.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	911.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1187.00		NIST Webbook

ripol	1217.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1215.00		NIST Webbook
sl	305.01	J/mol×K	NIST Webbook
tb	427.20	K	NIST Webbook
tb	427.20	K	NIST Webbook
tb	425.20	K	NIST Webbook
tb	427.00 ± 1.50	K	NIST Webbook
tc	642.00	K	NIST Webbook
tf	171.40	K	Aqueous Solubility Prediction Method
tf	172.00 ± 0.20	K	NIST Webbook
tt	171.64 ± 0.02	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.81	J/mol×K	428.48	Joback Method
cpg	185.27	J/mol×K	464.85	Joback Method
cpg	194.36	J/mol×K	501.21	Joback Method
cpg	203.07	J/mol×K	537.58	Joback Method
cpg	211.40	J/mol×K	573.94	Joback Method
cpg	219.35	J/mol×K	610.31	Joback Method
cpg	226.91	J/mol×K	646.67	Joback Method
cpl	204.01	J/mol×K	298.15	NIST Webbook
hfust	9.40	kJ/mol	171.64	NIST Webbook
hfust	9.40	kJ/mol	171.60	NIST Webbook
hfust	9.40	kJ/mol	171.60	NIST Webbook
hvapt	41.50	kJ/mol	396.00	NIST Webbook
hvapt	45.70	kJ/mol	360.50	NIST Webbook
hvapt	37.58	kJ/mol	427.20	NIST Webbook
hvapt	40.90 ± 0.10	kJ/mol	373.73	NIST Webbook

hvapt	40.90	kJ/mol	402.00	NIST Webbook
pvap	15.80	kPa	366.97	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	24.10	kPa	378.82	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	32.30	kPa	387.59	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	44.40	kPa	397.84	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	52.80	kPa	403.31	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	62.20	kPa	408.91	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	71.10	kPa	413.59	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K

pvap	82.10	kPa	418.73	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	90.50	kPa	422.25	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
pvap	100.70	kPa	426.39	Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 368.15 K
sfust	54.79	J/mol×K	171.64	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48234e+01
Coeff. B	-3.92063e+03
Coeff. C	-4.10150e+01
Temperature range (K), min.	310.74
Temperature range (K), max.	453.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.72140e+01
Coeff. B	-7.89627e+03
Coeff. C	-9.07739e+00
Coeff. D	4.78576e-06
Temperature range (K), min.	171.63
Temperature range (K), max.	642.00

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 303.15 K:	https://www.doi.org/10.1016/j.fluid.2010.02.043
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number structures, and solvent chemistry on solubility:	https://www.doi.org/10.1016/j.fluid.2004.10.021
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1826.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110816&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=1826
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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
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
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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