Diisopropyl sulfide

Other names:	(i-C3H7)2S
	2,2'-Thiobispropane
	2,4-Dimethyl-3-thiapentane
	DI-ISO-PROPYL SULFIDE
	Diisopropyl sulphide
	Isopropyl sulfide
	Propane, 2,2'-thiobis-
	diisopropylsulfide
Inchi:	InChI=1S/C6H14S/c1-5(2)7-6(3)4/h5-6H,1-4H3
InchiKey:	XYWDPYKBIRQXQS-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CC(C)SC(C)C
Mol. weight [g/mol]:	118.24
CAS:	625-80-9

Physical Properties

Property code	Value	Unit	Source
affp	876.40	kJ/mol	NIST Webbook
basg	846.60	kJ/mol	NIST Webbook
chl	-4782.77 ± 0.84	kJ/mol	NIST Webbook
chl	-4781.70 ± 2.00	kJ/mol	NIST Webbook
gf	27.88	kJ/mol	Joback Method
hf	-142.00 ± 1.30	kJ/mol	NIST Webbook
hf	-141.50	kJ/mol	NIST Webbook
hf	-143.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-181.10 ± 0.96	kJ/mol	NIST Webbook
hfl	-182.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.38	kJ/mol	Joback Method
hvap	39.60 ± 0.80	kJ/mol	NIST Webbook
hvap	39.64	kJ/mol	NIST Webbook
hvap	39.10	kJ/mol	NIST Webbook
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
hvap	39.60 ± 0.10	kJ/mol	NIST Webbook
hvap	39.60 ± 0.20	kJ/mol	NIST Webbook
hvap	39.00	kJ/mol	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.20 ± 0.20	eV	NIST Webbook

ie	8.00	eV	NIST Webbook
ie	8.25 ± 0.01	eV	NIST Webbook
ie	8.38 ± 0.05	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
log10ws	-2.24		Estimated Solubility Method
log10ws	-2.24		Aqueous Solubility Prediction Method
logp	2.536		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	788.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	778.00		NIST Webbook
sl	313.05	J/mol×K	NIST Webbook
tb	393.00 ± 4.00	K	NIST Webbook
tb	393.20	K	NIST Webbook
tb	393.20	K	NIST Webbook
tb	393.65 ± 0.50	K	NIST Webbook
tb	393.00 ± 2.00	K	NIST Webbook
tb	393.00 ± 0.30	K	NIST Webbook
tb	412.50 ± 0.60	K	NIST Webbook
tb	393.00 ± 2.00	K	NIST Webbook
tc	602.65	K	Joback Method
tf	195.07 ± 0.10	K	NIST Webbook
tf	181.10	K	Aqueous Solubility Prediction Method
tt	195.07 ± 0.01	K	NIST Webbook
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.72	J/mol×K	569.63	Joback Method
cpg	206.45	J/mol×K	404.58	Joback Method
cpg	218.68	J/mol×K	437.59	Joback Method
cpg	230.42	J/mol×K	470.60	Joback Method
cpg	241.66	J/mol×K	503.61	Joback Method

cpg	252.43	J/mol×K	536.62	Joback Method
cpg	272.54	J/mol×K	602.65	Joback Method
cpl	232.00	J/mol×K	298.15	NIST Webbook
hfust	10.42	kJ/mol	195.10	NIST Webbook
hfust	10.41	kJ/mol	195.07	NIST Webbook
hfust	10.42	kJ/mol	195.10	NIST Webbook
hvapt	37.40	kJ/mol	365.00	NIST Webbook
hvapt	39.40	kJ/mol	356.50	NIST Webbook
hvapt	37.70	kJ/mol	378.50	NIST Webbook
hvapt	33.80	kJ/mol	393.20	NIST Webbook
hvapt	38.50	kJ/mol	315.50	NIST Webbook
sfust	53.39	J/mol×K	195.07	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44790e+01
Coeff. B	-3.40729e+03
Coeff. C	-5.04570e+01
Temperature range (K), min.	290.55
Temperature range (K), max.	422.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.88044e+01
Coeff. B	-7.67655e+03
Coeff. C	-1.10212e+01
Coeff. D	7.64446e-06
Temperature range (K), min.	286.15

Temperature range (K), max.	585.71

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625809&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1837
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1837.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume