Disulfide, bis(1-methylethyl)

Other names:	Isopropyl disulfide
	Diisopropyl disulfide
	(i-C3H7S)2
	2,5-Dimethyl-3,4-dithiahexane
	Diisopropyl disulphide
	bis(1-Methylethyl) disulphide
	bis(1-methylethyl) disulphide (isopropyldisulphide)
	diisopropyl sulphide
Inchi:	InChI=1S/C6H14S2/c1-5(2)7-8-6(3)4/h5-6H,1-4H3
InchiKey:	LZAZXBXPKRULLB-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CC(C)SSC(C)C
Mol. weight [g/mol]:	150.31
CAS:	4253-89-8

Physical Properties

Property code	Value	Unit	Source
gf	61.00	kJ/mol	Joback Method
hf	-93.99	kJ/mol	Joback Method
hfus	12.51	kJ/mol	Joback Method
hvap	39.60	kJ/mol	NIST Webbook
hvap	49.30	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
log10ws	-3.32		Crippen Method
logp	3.185		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1023.00		NIST Webbook

rinpol	1018.00		NIST Webbook
rinpol	1016.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1252.00		NIST Webbook
tb	450.40	K	NIST Webbook
tb	447.00 ± 1.50	K	NIST Webbook
tb	447.00 ± 4.00	K	NIST Webbook
tb	448.70	K	NIST Webbook
tc	695.84	K	Joback Method
tf	204.10 ± 0.20	K	NIST Webbook
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.40	J/mol×K	473.36	Joback Method
cpg	267.47	J/mol×K	510.44	Joback Method
cpg	279.93	J/mol×K	547.52	Joback Method
cpg	291.77	J/mol×K	584.60	Joback Method
cpg	303.01	J/mol×K	621.68	Joback Method
cpg	313.64	J/mol×K	658.76	Joback Method
cpg	323.66	J/mol×K	695.84	Joback Method
hvapt	43.80	kJ/mol	412.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4253898&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume