Disulfide, bis(2-methylpropyl)

Other names:	Isobutyl disulfide
	Diisobutyl disulfide
	Bis(2-methylpropyl) disulphide
	2,7-Dimethyl-4,5-dithiaoctane
	Di(2-methylpropyl) disulfide
	diisobutyl disulphide
Inchi:	InChI=1S/C8H18S2/c1-7(2)5-9-10-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	ONJROLGQWMBXAP-UHFFFAOYSA-N
Formula:	C8H18S2
SMILES:	CC(C)CSSCC(C)C
Mol. weight [g/mol]:	178.36
CAS:	1518-72-5

Physical Properties

Property code	Value	Unit	Source
chl	-6692.40 ± 1.20	kJ/mol	NIST Webbook
gf	77.84	kJ/mol	Joback Method
hf	-170.90 ± 2.20	kJ/mol	NIST Webbook
hfl	-232.80 ± 1.40	kJ/mol	NIST Webbook
hfus	17.69	kJ/mol	Joback Method
hvap	57.20	kJ/mol	NIST Webbook
hvap	57.20 ± 0.10	kJ/mol	NIST Webbook
hvap	62.00 ± 2.00	kJ/mol	NIST Webbook
hvap	61.90	kJ/mol	NIST Webbook
log10ws	-3.45		Crippen Method
logp	3.680		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1205.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1178.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1435.00		NIST Webbook

tb	493.00 ± 15.00	K	NIST Webbook
tc	734.48	K	Joback Method
tf	218.72	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.26	J/mol×K	519.12	Joback Method
cpg	356.56	J/mol×K	555.01	Joback Method
cpg	371.10	J/mol×K	590.91	Joback Method
cpg	384.91	J/mol×K	626.80	Joback Method
cpg	397.97	J/mol×K	662.70	Joback Method
cpg	410.31	J/mol×K	698.59	Joback Method
cpg	421.93	J/mol×K	734.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1518725&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas 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
hvap: Enthalpy of vaporization at standard conditions
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