

Methyl isobutyl disulphide

Other names:	Methyl i-butyl disulfide Disulfide, methyl 2-methylpropyl 2-Methyl-4,5-dithiahexane Isobutyl methyl disulfide Disulfide, isobutyl methyl Methyl 2-methylpropyl disulfide
Inchi:	InChI=1S/C5H12S2/c1-5(2)4-7-6-3/h5H,4H2,1-3H3
InchiKey:	JQMZTHKFCOSKU-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CSSCC(C)C
Mol. weight [g/mol]:	136.28
CAS:	67421-83-4

Physical Properties

Property code	Value	Unit	Source
gf	55.02	kJ/mol	Joback Method
hf	-68.07	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.654		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1280.00		NIST Webbook
tb	450.92	K	Joback Method
tc	671.44	K	Joback Method
tf	199.91	K	Joback Method
vc	0.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.94	J/mol×K	450.92	Joback Method
cpg	225.27	J/mol×K	487.67	Joback Method
cpg	236.10	J/mol×K	524.43	Joback Method
cpg	246.44	J/mol×K	561.18	Joback Method
cpg	256.29	J/mol×K	597.94	Joback Method
cpg	265.64	J/mol×K	634.69	Joback Method
cpg	274.48	J/mol×K	671.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67421834&Units=SI

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
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

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