Disulfide, isopentyl methyl

Other names:	Methyl isopentyl disulphide
	Methyl i-amyl disulfide
	Disulfide, methyl 3-methylbutyl
	2-Methyl-5,6-dithiaheptane
	Isopentyl methyl disulfide
	Methyl isopentyl disulfide
	Isoamyl methyl disulfide
Inchi:	InChI=1S/C6H14S2/c1-6(2)4-5-8-7-3/h6H,4-5H2,1-3H3
InchiKey:	XTTOMWDBKHINLK-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CSSCCC(C)C
Mol. weight [g/mol]:	150.31
CAS:	72437-56-0

Physical Properties

Property code	Value	Unit	Source
gf	63.44	kJ/mol	Joback Method
hf	-88.71	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	42.20	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	3.044		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1411.00		NIST Webbook
ripol	1411.00		NIST Webbook
tb	473.80	K	Joback Method
tc	691.06	K	Joback Method
tf	211.18	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.21	J/mol×K	473.80	Joback Method
cpg	266.88	J/mol×K	510.01	Joback Method
cpg	278.98	J/mol×K	546.22	Joback Method
cpg	290.51	J/mol×K	582.43	Joback Method
cpg	301.47	J/mol×K	618.64	Joback Method
cpg	311.87	J/mol×K	654.85	Joback Method
cpg	321.69	J/mol×K	691.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72437560&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

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