Methyl (2,2-dimethylpropyl) sulfide

Other names: Propane, 2,2-dimethyl-1-(methylthio)-
Inchi: InChI=1S/C6H14S/c1-6(2,3)5-7-4/h5H2,1-4H3
InchiKey: YUFAJXXIXSYTMS-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CSCC(C)(C)C
Mol. weight [g/mol]: 118.24
CAS: 6079-57-8

Physical Properties

Property code	Value	Unit	Source
gf	35.60	kJ/mol	Joback Method
hf	-134.05	kJ/mol	Joback Method
hfus	8.01	kJ/mol	Joback Method
hvap	34.47	kJ/mol	Joback Method
ie	8.46 ± 0.05	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	2.396		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	823.00		NIST Webbook
tb	402.23	K	Joback Method
tc	604.13	K	Joback Method
tf	194.20	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.29	J/mol×K	402.23	Joback Method
cpg	221.25	J/mol×K	435.88	Joback Method
cpg	233.54	J/mol×K	469.53	Joback Method
cpg	245.18	J/mol×K	503.18	Joback Method
cpg	256.20	J/mol×K	536.83	Joback Method
cpg	266.61	J/mol×K	570.48	Joback Method

cpg	276.44	J/mol×K	604.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6079578&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume