S-methyl-2-methylthiobutanoate

Inchi: InChI=1S/C6H12OS2/c1-4-5(8-2)6(7)9-3/h5H,4H2,1-3H3
InchiKey: SEXRBODMANPKKE-UHFFFAOYSA-N
Formula: C6H12OS2
SMILES: CCC(SC)C(=O)SC
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	-65.48	kJ/mol	Joback Method
hf	-201.29	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.018		Crippen Method
mcvol	129.670	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	527.67	K	Joback Method
tc	754.80	K	Joback Method
tf	261.11	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.32	J/mol×K	527.67	Joback Method
cpg	281.07	J/mol×K	565.52	Joback Method
cpg	292.21	J/mol×K	603.38	Joback Method
cpg	302.74	J/mol×K	641.23	Joback Method
cpg	312.64	J/mol×K	679.09	Joback Method
cpg	321.93	J/mol×K	716.94	Joback Method
cpg	330.60	J/mol×K	754.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R274945&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume