S-Methyl 2-methylbutanethioate

Inchi: InChI=1S/C6H12OS/c1-4-5(2)6(7)8-3/h5H,4H2,1-3H3
InchiKey: IAMIOPHEADLKFT-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CCC(C)C(=O)SC
Mol. weight [g/mol]: 132.22
CAS: 42075-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-98.60	kJ/mol	Joback Method
hf	-243.16	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.922		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
ripol	1225.00		NIST Webbook
ripol	1225.00		NIST Webbook
tb	458.89	K	Joback Method
tc	664.31	K	Joback Method
tf	226.71	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.57	J/mol×K	458.89	Joback Method
cpg	234.76	J/mol×K	493.13	Joback Method
cpg	245.45	J/mol×K	527.36	Joback Method
cpg	255.64	J/mol×K	561.60	Joback Method
cpg	265.35	J/mol×K	595.83	Joback Method
cpg	274.58	J/mol×K	630.07	Joback Method
cpg	283.32	J/mol×K	664.31	Joback Method

Sources

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=C42075456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume