3-Mercapto-3-methylbutylthioformate

Inchi: InChI=1S/C6H12OS2/c1-6(2,8)3-4-9-5-7/h5,8H,3-4H2,1-2H3
InchiKey: ISYVLZOONZQKJL-UHFFFAOYSA-N
Formula: C6H12OS2
SMILES: CC(C)(S)CCSC=O
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	-34.53	kJ/mol	Joback Method
hf	-181.15	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	47.93	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	2.008		Crippen Method
mcvol	129.670	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	1023.00		NIST Webbook
tb	513.75	K	Joback Method
tc	745.18	K	Joback Method
tf	272.66	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.31	J/mol×K	513.75	Joback Method
cpg	284.22	J/mol×K	552.32	Joback Method
cpg	295.32	J/mol×K	590.89	Joback Method
cpg	305.65	J/mol×K	629.47	Joback Method
cpg	315.25	J/mol×K	668.04	Joback Method
cpg	324.15	J/mol×K	706.61	Joback Method
cpg	332.40	J/mol×K	745.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R598919&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume