3-methyl-3-sulfanylbutanal

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

Physical Properties

Property code	Value	Unit	Source
gf	-63.92	kJ/mol	Joback Method
hf	-219.63	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	41.19	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.717		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	450.89	K	Joback Method
tc	659.46	K	Joback Method
tf	236.20	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.94	J/mol×K	450.89	Joback Method
cpg	239.61	J/mol×K	485.65	Joback Method
cpg	250.62	J/mol×K	520.41	Joback Method
cpg	260.97	J/mol×K	555.17	Joback Method
cpg	270.71	J/mol×K	589.94	Joback Method
cpg	279.85	J/mol×K	624.70	Joback Method
cpg	288.43	J/mol×K	659.46	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=R419777&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
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