3-Methyl-3-sulfanylbutanal

Inchi: InChI=1S/C5H10OS/c1-5(2,7)3-4-6/h4,7H,3H2,1-2H3
InchiKey: WHGAWTZRCJEVHB-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CC(C)(S)CC=O
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-76.07	kJ/mol	Joback Method
hf	-202.38	kJ/mol	Joback Method
hfus	7.62	kJ/mol	Joback Method
hvap	38.89	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.284		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	845.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	422.09	K	Joback Method
tc	633.30	K	Joback Method
tf	226.99	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.86	J/mol×K	422.09	Joback Method
cpg	198.26	J/mol×K	457.29	Joback Method
cpg	208.00	J/mol×K	492.49	Joback Method
cpg	217.11	J/mol×K	527.69	Joback Method

cpg	225.63	J/mol×K	562.90	Joback Method
cpg	233.59	J/mol×K	598.10	Joback Method
cpg	241.01	J/mol×K	633.30	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=R609920&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