2-Methyl-2-(methyldithio)propanal

Other names: 2-methyl-2-(methyldithio)propionaldehyde
Inchi: InChI=1S/C5H10OS2/c1-5(2,4-6)8-7-3/h4H,1-3H3
InchiKey: VLBWEJJOETYCSE-UHFFFAOYSA-N
Formula: C5H10OS2
SMILES: CSSC(C)(C)C=O
Mol. weight [g/mol]: 150.26

Physical Properties

Property code	Value	Unit	Source
gf	-39.22	kJ/mol	Joback Method
hf	-157.12	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.975		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	496.79	K	Joback Method
tc	732.11	K	Joback Method
tf	259.33	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.24	J/mol×K	496.79	Joback Method
cpg	243.02	J/mol×K	536.01	Joback Method
cpg	253.08	J/mol×K	575.23	Joback Method
cpg	262.46	J/mol×K	614.45	Joback Method
cpg	271.17	J/mol×K	653.67	Joback Method
cpg	279.23	J/mol×K	692.89	Joback Method

cpg	286.68	J/mol×K	732.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67952607&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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