3-Mercapto-butyraldehyde

Other names: 3-mercaptobutanal
Inchi: InChI=1S/C4H8OS/c1-4(6)2-3-5/h3-4,6H,2H2,1H3
InchiKey: USJRMLZTONLKON-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: CC(S)CC=O
Mol. weight [g/mol]: 104.17

Physical Properties

Property code	Value	Unit	Source
gf	-89.77	kJ/mol	Joback Method
hf	-178.27	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	37.57	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.894		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	840.00		NIST Webbook
tb	402.00	K	Joback Method
tc	606.28	K	Joback Method
tf	198.30	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.49	J/mol×K	402.00	Joback Method
cpg	157.46	J/mol×K	436.05	Joback Method
cpg	165.07	J/mol×K	470.09	Joback Method
cpg	172.31	J/mol×K	504.14	Joback Method
cpg	179.19	J/mol×K	538.18	Joback Method

cpg	185.73	J/mol×K	572.23	Joback Method
cpg	191.94	J/mol×K	606.28	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=R205568&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume