Propanal, 2-methylthio

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

Physical Properties

Property code	Value	Unit	Source
gf	-86.04	kJ/mol	Joback Method
hf	-174.88	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.937		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	885.00		NIST Webbook
ripol	1426.00		NIST Webbook
tb	407.92	K	Joback Method
tc	612.32	K	Joback Method
tf	196.24	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.36	J/mol×K	407.92	Joback Method
cpg	158.35	J/mol×K	441.99	Joback Method
cpg	166.02	J/mol×K	476.05	Joback Method
cpg	173.36	J/mol×K	510.12	Joback Method
cpg	180.37	J/mol×K	544.19	Joback Method

cpg	187.06	J/mol×K	578.26	Joback Method
cpg	193.42	J/mol×K	612.32	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=R87651&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