Hexanal, 3-(methylthio)

Other names: 3-(methylthio)hexanal
Inchi: InChI=1S/C7H14OS/c1-3-4-7(9-2)5-6-8/h6-7H,3-5H2,1-2H3
InchiKey: VIVJHDGDCOQORO-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCC(CC=O)SC
Mol. weight [g/mol]: 146.25
CAS: 38433-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-60.78	kJ/mol	Joback Method
hf	-236.80	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.107		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	476.56	K	Joback Method
tc	674.08	K	Joback Method
tf	230.05	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.02	J/mol×K	476.56	Joback Method
cpg	278.06	J/mol×K	509.48	Joback Method
cpg	289.55	J/mol×K	542.40	Joback Method
cpg	300.51	J/mol×K	575.32	Joback Method
cpg	310.96	J/mol×K	608.24	Joback Method
cpg	320.89	J/mol×K	641.16	Joback Method

cpg	330.31	J/mol×K	674.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38433748&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume