Propanoic acid, 3-(methylthio)-

Other names:	Propionic acid, 3-(methylthio)-
	3-(Methylthio)propanoic acid
	3-(Methylthio)propionic acid
	4-Thiapentanoic acid
Inchi:	InChI=1S/C4H8O2S/c1-7-3-2-4(5)6/h2-3H2,1H3,(H,5,6)
InchiKey:	CAOMCZAIALVUPA-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	CSCCC(=O)O
Mol. weight [g/mol]:	120.17
CAS:	646-01-5

Physical Properties

Property code	Value	Unit	Source
gf	-249.82	kJ/mol	Joback Method
hf	-348.83	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.824		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1150.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2320.00		NIST Webbook
tb	505.75	K	Joback Method
tc	699.71	K	Joback Method
tf	279.99	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.77	J/mol×K	505.75	Joback Method
cpg	191.87	J/mol×K	538.08	Joback Method
cpg	198.65	J/mol×K	570.40	Joback Method
cpg	205.12	J/mol×K	602.73	Joback Method
cpg	211.28	J/mol×K	635.05	Joback Method
cpg	217.13	J/mol×K	667.38	Joback Method
cpg	222.68	J/mol×K	699.71	Joback Method

Sources

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=C646015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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