Thiomethyl ester «alpha»-(methyl-thio)propionic acid

Inchi: InChI=1S/C5H10OS2/c1-4(7-2)5(6)8-3/h4H,1-3H3
InchiKey: NGIPHAZKKJGVHC-UHFFFAOYSA-N
Formula: C5H10OS2
SMILES: CSC(=O)C(C)SC
Mol. weight [g/mol]: 150.26

Physical Properties

Property code	Value	Unit	Source
gf	-73.90	kJ/mol	Joback Method
hf	-180.65	kJ/mol	Joback Method
hfus	15.04	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.627		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1036.00		NIST Webbook
tb	504.79	K	Joback Method
tc	736.10	K	Joback Method
tf	249.84	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.20	J/mol×K	504.79	Joback Method
cpg	237.70	J/mol×K	543.34	Joback Method
cpg	247.67	J/mol×K	581.89	Joback Method
cpg	257.10	J/mol×K	620.45	Joback Method
cpg	265.98	J/mol×K	659.00	Joback Method
cpg	274.32	J/mol×K	697.55	Joback Method
cpg	282.10	J/mol×K	736.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157796&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