L-Methionine, methyl ester

Other names: methyl methionate
Inchi: InChI=1S/C6H13NO2S/c1-9-6(8)5(7)3-4-10-2/h5H,3-4,7H2,1-2H3/t5-/m1/s1
InchiKey: UIHPNZDZCOEZEN-RXMQYKEDSA-N
Formula: C6H13NO2S
SMILES: COC(=O)C(N)CCSC
Mol. weight [g/mol]: 163.24
CAS: 10332-17-9

Physical Properties

Property code	Value	Unit	Source
gf	-137.15	kJ/mol	Joback Method
hf	-341.59	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.240		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1289.50		NIST Webbook
rinpol	1289.50		NIST Webbook
tb	553.84	K	Joback Method
tc	767.87	K	Joback Method
tf	332.20	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.93	J/mol×K	553.84	Joback Method
cpg	309.33	J/mol×K	589.51	Joback Method
cpg	320.17	J/mol×K	625.18	Joback Method
cpg	330.46	J/mol×K	660.86	Joback Method
cpg	340.20	J/mol×K	696.53	Joback Method
cpg	349.36	J/mol×K	732.20	Joback Method

cpg	357.95	J/mol×K	767.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10332179&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