L-Methionine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C9H14ClF2NO3S/c1-3-16-7(14)6(4-5-17-2)13-8(15)9(10,11)12/h6H,3-5H2,1-2
InchiKey: OMNSGFAPMYNXHD-UHFFFAOYSA-N
Formula: C9H14ClF2NO3S
SMILES: CCOC(=O)C(CCSC)NC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 289.73

Physical Properties

Property code	Value	Unit	Source
gf	-616.58	kJ/mol	Joback Method
hf	-913.12	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.619		Crippen Method
mcvol	188.790	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	686.73	K	Joback Method
tc	887.58	K	Joback Method
tf	418.86	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.28	J/mol×K	686.73	Joback Method
cpg	501.58	J/mol×K	720.21	Joback Method
cpg	512.12	J/mol×K	753.68	Joback Method
cpg	521.91	J/mol×K	787.16	Joback Method
cpg	530.97	J/mol×K	820.63	Joback Method
cpg	539.33	J/mol×K	854.11	Joback Method
cpg	547.00	J/mol×K	887.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375645&Units=SI

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