l-Methionine, N-(5-chlorovaleryl)-, methyl ester

Inchi: InChI=1S/C11H20ClNO3S/c1-16-11(15)9(6-8-17-2)13-10(14)5-3-4-7-12/h9H,3-8H2,1-2H
InchiKey: IQLBEONWSITFOW-UHFFFAOYSA-N
Formula: C11H20ClNO3S
SMILES: COC(=O)C(CCSC)NC(=O)CCCCCl
Mol. weight [g/mol]: 281.80

Physical Properties

Property code	Value	Unit	Source
gf	-212.96	kJ/mol	Joback Method
hf	-553.43	kJ/mol	Joback Method
hfus	38.53	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.806		Crippen Method
mcvol	213.430	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2076.00		NIST Webbook
tb	737.18	K	Joback Method
tc	939.71	K	Joback Method
tf	437.80	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.73	J/mol×K	737.18	Joback Method
cpg	588.79	J/mol×K	770.93	Joback Method
cpg	601.02	J/mol×K	804.69	Joback Method
cpg	612.41	J/mol×K	838.44	Joback Method
cpg	622.97	J/mol×K	872.20	Joback Method
cpg	632.72	J/mol×K	905.95	Joback Method
cpg	641.67	J/mol×K	939.71	Joback Method

Sources

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=U299718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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