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

Inchi: InChI=1S/C9H16ClNO3/c1-7(9(13)14-2)11-8(12)5-3-4-6-10/h7H,3-6H2,1-2H3,(H,11,12)
InchiKey: XARKWCNFPJCPGN-UHFFFAOYSA-N
Formula: C9H16ClNO3
SMILES: COC(=O)C(C)NC(=O)CCCCCl
Mol. weight [g/mol]: 221.68

Physical Properties

Property code	Value	Unit	Source
gf	-262.92	kJ/mol	Joback Method
hf	-554.02	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.073		Crippen Method
mcvol	168.900	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	622.64	K	Joback Method
tc	814.83	K	Joback Method
tf	380.86	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.91	J/mol×K	622.64	Joback Method
cpg	432.16	J/mol×K	654.67	Joback Method
cpg	443.77	J/mol×K	686.70	Joback Method
cpg	454.77	J/mol×K	718.73	Joback Method
cpg	465.15	J/mol×K	750.77	Joback Method
cpg	474.92	J/mol×K	782.80	Joback Method
cpg	484.10	J/mol×K	814.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299713&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

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