D-Alanine, N-(5-chlorovaleryl)-, pentyl ester

Inchi: InChI=1S/C13H24ClNO3/c1-3-4-7-10-18-13(17)11(2)15-12(16)8-5-6-9-14/h11H,3-10H2,1
InchiKey: FSKCEGKRZVKHRS-UHFFFAOYSA-N
Formula: C13H24ClNO3
SMILES: CCCCCOC(=O)C(C)NC(=O)CCCCCl
Mol. weight [g/mol]: 277.79

Physical Properties

Property code	Value	Unit	Source
gf	-229.24	kJ/mol	Joback Method
hf	-636.58	kJ/mol	Joback Method
hfus	39.59	kJ/mol	Joback Method
hvap	70.87	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.634		Crippen Method
mcvol	225.260	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	714.16	K	Joback Method
tc	900.44	K	Joback Method
tf	425.94	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.34	J/mol×K	714.16	Joback Method
cpg	641.79	J/mol×K	745.21	Joback Method
cpg	655.46	J/mol×K	776.25	Joback Method
cpg	668.36	J/mol×K	807.30	Joback Method
cpg	680.51	J/mol×K	838.35	Joback Method
cpg	691.93	J/mol×K	869.40	Joback Method
cpg	702.62	J/mol×K	900.44	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=U348480&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