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

Inchi: InChI=1S/C15H28ClNO3/c1-3-4-5-6-9-12-20-15(19)13(2)17-14(18)10-7-8-11-16/h13H,3-
InchiKey: KOFVZRFXZTVRON-UHFFFAOYSA-N
Formula: C15H28ClNO3
SMILES: CCCCCCCOC(=O)C(C)NC(=O)CCCCCl
Mol. weight [g/mol]: 305.84

Physical Properties

Property code	Value	Unit	Source
gf	-212.40	kJ/mol	Joback Method
hf	-677.86	kJ/mol	Joback Method
hfus	44.77	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.414		Crippen Method
mcvol	253.440	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	759.92	K	Joback Method
tc	945.97	K	Joback Method
tf	448.48	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.55	J/mol×K	759.92	Joback Method
cpg	753.83	J/mol×K	790.93	Joback Method
cpg	768.25	J/mol×K	821.94	Joback Method
cpg	781.83	J/mol×K	852.94	Joback Method
cpg	794.59	J/mol×K	883.95	Joback Method
cpg	806.55	J/mol×K	914.96	Joback Method
cpg	817.74	J/mol×K	945.97	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=U348483&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