D-Alanine, N-(2-chlorobenzoyl)-, propyl ester

Inchi: InChI=1S/C13H16ClNO3/c1-3-8-18-13(17)9(2)15-12(16)10-6-4-5-7-11(10)14/h4-7,9H,3,8
InchiKey: VGTRQCWOAIEZNT-UHFFFAOYSA-N
Formula: C13H16ClNO3
SMILES: CCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 269.72

Physical Properties

Property code	Value	Unit	Source
gf	-126.46	kJ/mol	Joback Method
hf	-411.52	kJ/mol	Joback Method
hfus	33.24	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.412		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	2035.00		NIST Webbook
tb	745.82	K	Joback Method
tc	963.08	K	Joback Method
tf	464.88	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.42	J/mol×K	745.82	Joback Method
cpg	552.29	J/mol×K	782.03	Joback Method
cpg	564.20	J/mol×K	818.24	Joback Method
cpg	575.20	J/mol×K	854.45	Joback Method
cpg	585.31	J/mol×K	890.66	Joback Method
cpg	594.55	J/mol×K	926.87	Joback Method
cpg	602.95	J/mol×K	963.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354069&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