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

Inchi: InChI=1S/C12H14ClNO3/c1-3-17-12(16)8(2)14-11(15)9-6-4-5-7-10(9)13/h4-8H,3H2,1-2H
InchiKey: FIGHCVBYPAFJIP-UHFFFAOYSA-N
Formula: C12H14ClNO3
SMILES: CCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 255.70

Physical Properties

Property code	Value	Unit	Source
gf	-134.88	kJ/mol	Joback Method
hf	-390.88	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.021		Crippen Method
mcvol	187.410	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1937.00		NIST Webbook
tb	722.94	K	Joback Method
tc	943.45	K	Joback Method
tf	453.61	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.97	J/mol×K	722.94	Joback Method
cpg	499.38	J/mol×K	759.69	Joback Method
cpg	510.88	J/mol×K	796.44	Joback Method
cpg	521.49	J/mol×K	833.20	Joback Method
cpg	531.24	J/mol×K	869.95	Joback Method
cpg	540.13	J/mol×K	906.70	Joback Method
cpg	548.21	J/mol×K	943.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354068&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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