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

Inchi: InChI=1S/C14H18ClNO3/c1-3-4-9-19-14(18)10(2)16-13(17)11-7-5-6-8-12(11)15/h5-8,10
InchiKey: AIJHHKQKRLVNEK-UHFFFAOYSA-N
Formula: C14H18ClNO3
SMILES: CCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 283.75

Physical Properties

Property code	Value	Unit	Source
gf	-118.04	kJ/mol	Joback Method
hf	-432.16	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	76.03	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.802		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	768.70	K	Joback Method
tc	983.20	K	Joback Method
tf	476.15	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.04	J/mol×K	768.70	Joback Method
cpg	606.28	J/mol×K	804.45	Joback Method
cpg	618.55	J/mol×K	840.20	Joback Method
cpg	629.87	J/mol×K	875.95	Joback Method
cpg	640.29	J/mol×K	911.70	Joback Method
cpg	649.82	J/mol×K	947.45	Joback Method
cpg	658.49	J/mol×K	983.20	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=U354070&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