D-Alanine, N-(3-chloro-2-fluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C14H17ClFNO3/c1-3-4-8-20-14(19)9(2)17-13(18)10-6-5-7-11(15)12(10)16/h5-

InchiKey: UHNAJCCMVAJVMF-UHFFFAOYSA-N

Formula: C14H17ClFNO3

SMILES: CCCCOC(=O)C(C)NC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 301.74

Physical Properties

Property code	Value	Unit	Source
gf	-322.48	kJ/mol	Joback Method
hf	-639.74	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	2.941		Crippen Method
mcvol	217.360	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2119.00		NIST Webbook
tb	772.95	K	Joback Method
tc	980.93	K	Joback Method
tf	489.26	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.53	J/mol×K	772.95	Joback Method
cpg	612.13	J/mol×K	807.61	Joback Method
cpg	623.84	J/mol×K	842.28	Joback Method
cpg	634.66	J/mol×K	876.94	Joback Method
cpg	644.63	J/mol×K	911.61	Joback Method
cpg	653.76	J/mol×K	946.27	Joback Method
cpg	662.07	J/mol×K	980.93	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=U348336&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