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

Inchi: InChI=1S/C15H19ClFNO3/c1-3-4-5-9-21-15(20)10(2)18-14(19)11-7-6-8-12(16)13(11)17/

InchiKey: YKUICNAPNCVSIH-UHFFFAOYSA-N

Formula: C15H19ClFNO3

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

Mol. weight [g/mol]: 315.77

Physical Properties

Property code	Value	Unit	Source
gf	-314.06	kJ/mol	Joback Method
hf	-660.38	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	78.10	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.331		Crippen Method
mcvol	231.450	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	795.83	K	Joback Method
tc	1002.26	K	Joback Method
tf	500.53	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.19	J/mol×K	795.83	Joback Method
cpg	667.15	J/mol×K	830.24	Joback Method
cpg	679.18	J/mol×K	864.64	Joback Method
cpg	690.29	J/mol×K	899.05	Joback Method
cpg	700.53	J/mol×K	933.45	Joback Method
cpg	709.90	J/mol×K	967.86	Joback Method
cpg	718.43	J/mol×K	1002.26	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=U348337&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