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

Inchi: InChI=1S/C15H20ClNO3/c1-3-4-7-10-20-15(19)11(2)17-14(18)12-8-5-6-9-13(12)16/h5-6
InchiKey: FYPGMHRRIZGXLQ-UHFFFAOYSA-N
Formula: C15H20ClNO3
SMILES: CCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 297.78

Physical Properties

Property code	Value	Unit	Source
gf	-109.62	kJ/mol	Joback Method
hf	-452.80	kJ/mol	Joback Method
hfus	38.42	kJ/mol	Joback Method
hvap	78.26	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.192		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	791.58	K	Joback Method
tc	1003.84	K	Joback Method
tf	487.42	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.73	J/mol×K	791.58	Joback Method
cpg	661.29	J/mol×K	826.96	Joback Method
cpg	673.86	J/mol×K	862.33	Joback Method
cpg	685.46	J/mol×K	897.71	Joback Method
cpg	696.13	J/mol×K	933.09	Joback Method
cpg	705.90	J/mol×K	968.47	Joback Method
cpg	714.79	J/mol×K	1003.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354071&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