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

Inchi: InChI=1S/C28H46ClNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-33-28(32)24(

InchiKey: GEXMJYGYKRVKTA-UHFFFAOYSA-N

Formula: C28H46ClNO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 480.12

Physical Properties

Property code	Value	Unit	Source
gf	-0.16	kJ/mol	Joback Method
hf	-721.12	kJ/mol	Joback Method
hfus	72.09	kJ/mol	Joback Method
hvap	107.19	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.263		Crippen Method
mcvol	412.850	ml/mol	McGowan Method
pc	817.73	kPa	Joback Method
rinpol	3595.00		NIST Webbook
tb	1089.02	K	Joback Method
tc	1343.17	K	Joback Method
tf	633.93	K	Joback Method
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.01	J/mol×K	1089.02	Joback Method
cpg	1444.31	J/mol×K	1131.38	Joback Method
cpg	1459.90	J/mol×K	1173.74	Joback Method
cpg	1473.91	J/mol×K	1216.09	Joback Method
cpg	1486.46	J/mol×K	1258.45	Joback Method
cpg	1497.67	J/mol×K	1300.81	Joback Method
cpg	1507.67	J/mol×K	1343.17	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=U354085&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