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

Inchi: InChI=1S/C27H44ClNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-32-27(31)23(2)2

InchiKey: DSWFDGCCCVYANX-UHFFFAOYSA-N

Formula: C27H44ClNO3

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

Mol. weight [g/mol]: 466.10

Physical Properties

Property code	Value	Unit	Source
gf	-8.58	kJ/mol	Joback Method
hf	-700.48	kJ/mol	Joback Method
hfus	69.50	kJ/mol	Joback Method
hvap	104.97	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	7.873		Crippen Method
mcvol	398.760	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
rinpol	3478.00		NIST Webbook
rinpol	3478.00		NIST Webbook
tb	1066.14	K	Joback Method
tc	1310.78	K	Joback Method
tf	622.66	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.95	J/mol×K	1066.14	Joback Method
cpg	1380.80	J/mol×K	1106.91	Joback Method
cpg	1396.05	J/mol×K	1147.69	Joback Method
cpg	1409.81	J/mol×K	1188.46	Joback Method
cpg	1422.18	J/mol×K	1229.24	Joback Method
cpg	1433.27	J/mol×K	1270.01	Joback Method
cpg	1443.18	J/mol×K	1310.78	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=U354084&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