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

Inchi: InChI=1S/C25H40ClNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-20-30-25(29)21(2)27-24(2

InchiKey: HHQZVTJISGQHTN-UHFFFAOYSA-N

Formula: C25H40ClNO3

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

Mol. weight [g/mol]: 438.04

Physical Properties

Property code	Value	Unit	Source
gf	-25.42	kJ/mol	Joback Method
hf	-659.20	kJ/mol	Joback Method
hfus	64.32	kJ/mol	Joback Method
hvap	100.52	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.093		Crippen Method
mcvol	370.580	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	1020.38	K	Joback Method
tc	1249.90	K	Joback Method
tf	600.12	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.95	J/mol×K	1020.38	Joback Method
cpg	1255.04	J/mol×K	1058.63	Joback Method
cpg	1269.71	J/mol×K	1096.89	Joback Method
cpg	1283.04	J/mol×K	1135.14	Joback Method
cpg	1295.11	J/mol×K	1173.39	Joback Method
cpg	1306.01	J/mol×K	1211.65	Joback Method
cpg	1315.79	J/mol×K	1249.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354082&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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