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

Inchi: InChI=1S/C22H34ClNO3/c1-3-4-5-6-7-8-9-10-11-14-17-27-22(26)18(2)24-21(25)19-15-1
InchiKey: WTLUIOCGSBSWMM-UHFFFAOYSA-N
Formula: C22H34ClNO3
SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 395.96

Physical Properties

Property code	Value	Unit	Source
gf	-50.68	kJ/mol	Joback Method
hf	-597.28	kJ/mol	Joback Method
hfus	56.55	kJ/mol	Joback Method
hvap	93.84	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.922		Crippen Method
mcvol	328.310	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	951.74	K	Joback Method
tc	1167.03	K	Joback Method
tf	566.31	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.82	J/mol×K	951.74	Joback Method
cpg	1070.04	J/mol×K	987.62	Joback Method
cpg	1084.03	J/mol×K	1023.50	Joback Method
cpg	1096.86	J/mol×K	1059.38	Joback Method
cpg	1108.56	J/mol×K	1095.27	Joback Method
cpg	1119.21	J/mol×K	1131.15	Joback Method
cpg	1128.84	J/mol×K	1167.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354079&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