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

Inchi: InChI=1S/C23H36ClNO3/c1-3-4-5-6-7-8-9-10-11-12-15-18-28-23(27)19(2)25-22(26)20-1
InchiKey: LLXLIEBIYGXQTJ-UHFFFAOYSA-N
Formula: C23H36ClNO3
SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 409.99

Physical Properties

Property code	Value	Unit	Source
gf	-42.26	kJ/mol	Joback Method
hf	-617.92	kJ/mol	Joback Method
hfus	59.14	kJ/mol	Joback Method
hvap	96.06	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.312		Crippen Method
mcvol	342.400	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	3064.00		NIST Webbook
rinpol	3064.00		NIST Webbook
tb	974.62	K	Joback Method
tc	1193.63	K	Joback Method
tf	577.58	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.69	J/mol×K	974.62	Joback Method
cpg	1131.17	J/mol×K	1011.12	Joback Method
cpg	1145.37	J/mol×K	1047.62	Joback Method
cpg	1158.35	J/mol×K	1084.12	Joback Method
cpg	1170.17	J/mol×K	1120.62	Joback Method
cpg	1180.90	J/mol×K	1157.12	Joback Method
cpg	1190.58	J/mol×K	1193.63	Joback Method

Sources

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=U354080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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