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

Inchi: InChI=1S/C20H30ClNO3/c1-3-4-5-6-7-8-9-12-15-25-20(24)16(2)22-19(23)17-13-10-11-1
InchiKey: RSIQHWCJHVROCB-UHFFFAOYSA-N
Formula: C20H30ClNO3
SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 367.91

Physical Properties

Property code	Value	Unit	Source
gf	-67.52	kJ/mol	Joback Method
hf	-556.00	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	89.39	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.142		Crippen Method
mcvol	300.130	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2741.00		NIST Webbook
tb	905.98	K	Joback Method
tc	1116.58	K	Joback Method
tf	543.77	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.82	J/mol×K	905.98	Joback Method
cpg	949.58	J/mol×K	941.08	Joback Method
cpg	963.20	J/mol×K	976.18	Joback Method
cpg	975.73	J/mol×K	1011.28	Joback Method
cpg	987.20	J/mol×K	1046.38	Joback Method
cpg	997.68	J/mol×K	1081.48	Joback Method
cpg	1007.19	J/mol×K	1116.58	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=U354077&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