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

Inchi: InChI=1S/C19H28ClNO3/c1-3-4-5-6-7-8-11-14-24-19(23)15(2)21-18(22)16-12-9-10-13-1
InchiKey: YKBDOMFIFYGLDM-UHFFFAOYSA-N
Formula: C19H28ClNO3
SMILES: CCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 353.88

Physical Properties

Property code	Value	Unit	Source
gf	-75.94	kJ/mol	Joback Method
hf	-535.36	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	87.16	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.752		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook
tb	883.10	K	Joback Method
tc	1092.61	K	Joback Method
tf	532.50	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.81	J/mol×K	883.10	Joback Method
cpg	890.35	J/mol×K	918.02	Joback Method
cpg	903.79	J/mol×K	952.94	Joback Method
cpg	916.16	J/mol×K	987.85	Joback Method
cpg	927.52	J/mol×K	1022.77	Joback Method
cpg	937.89	J/mol×K	1057.69	Joback Method
cpg	947.33	J/mol×K	1092.61	Joback Method

Sources

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=U354076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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