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

Inchi: InChI=1S/C18H26ClNO3/c1-3-4-5-6-7-10-13-23-18(22)14(2)20-17(21)15-11-8-9-12-16(1
InchiKey: OIXDLRASFXWLAP-UHFFFAOYSA-N
Formula: C18H26ClNO3
SMILES: CCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 339.86

Physical Properties

Property code	Value	Unit	Source
gf	-84.36	kJ/mol	Joback Method
hf	-514.72	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	84.94	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.362		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2537.00		NIST Webbook
tb	860.22	K	Joback Method
tc	1069.40	K	Joback Method
tf	521.23	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.53	J/mol×K	860.22	Joback Method
cpg	831.85	J/mol×K	895.08	Joback Method
cpg	845.10	J/mol×K	929.95	Joback Method
cpg	857.32	J/mol×K	964.81	Joback Method
cpg	868.54	J/mol×K	999.67	Joback Method
cpg	878.80	J/mol×K	1034.54	Joback Method
cpg	888.13	J/mol×K	1069.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354075&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