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

Inchi: InChI=1S/C17H24ClNO3/c1-3-4-5-6-9-12-22-17(21)13(2)19-16(20)14-10-7-8-11-15(14)1
InchiKey: CYUVDTMTBCCBQE-UHFFFAOYSA-N
Formula: C17H24ClNO3
SMILES: CCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 325.83

Physical Properties

Property code	Value	Unit	Source
gf	-92.78	kJ/mol	Joback Method
hf	-494.08	kJ/mol	Joback Method
hfus	43.60	kJ/mol	Joback Method
hvap	82.71	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.972		Crippen Method
mcvol	257.860	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2436.00		NIST Webbook
tb	837.34	K	Joback Method
tc	1046.90	K	Joback Method
tf	509.96	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.05	J/mol×K	837.34	Joback Method
cpg	774.14	J/mol×K	872.27	Joback Method
cpg	787.19	J/mol×K	907.19	Joback Method
cpg	799.23	J/mol×K	942.12	Joback Method
cpg	810.29	J/mol×K	977.05	Joback Method
cpg	820.41	J/mol×K	1011.97	Joback Method
cpg	829.63	J/mol×K	1046.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354074&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