L-Alanine, N-(2-chlorobenzoyl)-, methyl ester

Inchi: InChI=1S/C11H12ClNO3/c1-7(11(15)16-2)13-10(14)8-5-3-4-6-9(8)12/h3-7H,1-2H3,(H,13
InchiKey: IYECSIXZMPHUOA-UHFFFAOYSA-N
Formula: C11H12ClNO3
SMILES: COC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 241.67

Physical Properties

Property code	Value	Unit	Source
hf	-498.95	kJ/mol	Cheméo Relay (1.0)
hfus	28.06	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
logp	1.631		Crippen Method
mcvol	173.320	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1772.00		NIST Webbook
tb	567.49	K	Cheméo Relay (1.0)
tf	366.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.75	J/mol×K	700.06	Joback Method
cpg	447.64	J/mol×K	737.43	Joback Method
cpg	458.64	J/mol×K	774.80	Joback Method
cpg	468.79	J/mol×K	812.17	Joback Method
cpg	478.10	J/mol×K	849.54	Joback Method
cpg	486.59	J/mol×K	886.90	Joback Method
cpg	494.28	J/mol×K	924.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299586&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point