«beta»-Alanine, N-(2-chlorobenzoyl)-, ethyl ester

Inchi: InChI=1S/C12H14ClNO3/c1-2-17-11(15)7-8-14-12(16)9-5-3-4-6-10(9)13/h3-6H,2,7-8H2,1

InchiKey: SLITWDDTDLXMJU-UHFFFAOYSA-N

Formula: C12H14ClNO3

SMILES: CCOC(=O)CCNC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 255.70

Physical Properties

Property code	Value	Unit	Source
gf	-132.44	kJ/mol	Joback Method
hf	-385.60	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.023		Crippen Method
mcvol	187.410	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	723.38	K	Joback Method
tc	940.06	K	Joback Method
tf	468.61	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.38	J/mol×K	723.38	Joback Method
cpg	498.57	J/mol×K	759.49	Joback Method
cpg	509.88	J/mol×K	795.61	Joback Method
cpg	520.34	J/mol×K	831.72	Joback Method
cpg	529.98	J/mol×K	867.84	Joback Method
cpg	538.81	J/mol×K	903.95	Joback Method
cpg	546.86	J/mol×K	940.06	Joback Method

Sources

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=U321572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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