«beta»-Alanine, N-(4-chlorobenzoyl)-, butyl ester

Inchi: InChI=1S/C14H18ClNO3/c1-2-3-10-19-13(17)8-9-16-14(18)11-4-6-12(15)7-5-11/h4-7H,2

InchiKey: GQSWAGGIXFHPKC-UHFFFAOYSA-N

Formula: C14H18ClNO3

SMILES: CCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 283.75

Physical Properties

Property code	Value	Unit	Source
gf	-115.60	kJ/mol	Joback Method
hf	-426.88	kJ/mol	Joback Method
hfus	39.35	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.803		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	769.14	K	Joback Method
tc	980.40	K	Joback Method
tf	491.15	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.46	J/mol×K	769.14	Joback Method
cpg	605.49	J/mol×K	804.35	Joback Method
cpg	617.60	J/mol×K	839.56	Joback Method
cpg	628.80	J/mol×K	874.77	Joback Method
cpg	639.13	J/mol×K	909.98	Joback Method
cpg	648.61	J/mol×K	945.19	Joback Method
cpg	657.26	J/mol×K	980.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321718&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