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

Inchi: InChI=1S/C15H20ClNO3/c1-2-3-6-11-20-14(18)9-10-17-15(19)12-7-4-5-8-13(12)16/h4-5

InchiKey: MMWDKJCCDUDHPZ-UHFFFAOYSA-N

Formula: C15H20ClNO3

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

Mol. weight [g/mol]: 297.78

Physical Properties

Property code	Value	Unit	Source
gf	-107.18	kJ/mol	Joback Method
hf	-447.52	kJ/mol	Joback Method
hfus	41.94	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.193		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	2347.00		NIST Webbook
tb	792.02	K	Joback Method
tc	1001.35	K	Joback Method
tf	502.42	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.16	J/mol×K	792.02	Joback Method
cpg	660.53	J/mol×K	826.91	Joback Method
cpg	672.95	J/mol×K	861.80	Joback Method
cpg	684.45	J/mol×K	896.69	Joback Method
cpg	695.04	J/mol×K	931.58	Joback Method
cpg	704.77	J/mol×K	966.46	Joback Method
cpg	713.66	J/mol×K	1001.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321575&Units=SI

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