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

Inchi: InChI=1S/C15H20BrNO3/c1-2-3-6-11-20-14(18)9-10-17-15(19)12-7-4-5-8-13(12)16/h4-5

InchiKey: FZOGFAKYYHDDPC-UHFFFAOYSA-N

Formula: C15H20BrNO3

SMILES: CCCCCOC(=O)CCNC(=O)c1ccccc1Br

Mol. weight [g/mol]: 342.23

Physical Properties

Property code	Value	Unit	Source
gf	-80.93	kJ/mol	Joback Method
hf	-405.45	kJ/mol	Joback Method
hfus	43.03	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.302		Crippen Method
mcvol	234.940	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	820.75	K	Joback Method
tc	1036.51	K	Joback Method
tf	532.30	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.84	J/mol×K	820.75	Joback Method
cpg	671.75	J/mol×K	856.71	Joback Method
cpg	683.71	J/mol×K	892.67	Joback Method
cpg	694.76	J/mol×K	928.63	Joback Method
cpg	704.93	J/mol×K	964.59	Joback Method
cpg	714.26	J/mol×K	1000.55	Joback Method
cpg	722.80	J/mol×K	1036.51	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=U321729&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