

«beta»-Alanine, N-(3-bromobenzoyl)-, pentyl ester

Inchi:	InChI=1S/C15H20BrNO3/c1-2-3-4-10-20-14(18)8-9-17-15(19)12-6-5-7-13(16)11-12/h5-7
InchiKey:	ZRIKBCGLJWWFTM-UHFFFAOYSA-N
Formula:	C15H20BrNO3
SMILES:	CCCCCOC(=O)CCNC(=O)c1cccc(Br)c1
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
mvol	234.940	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	820.75	K	Joback Method
tc	1036.51	K	Joback Method
tf	532.30	K	Joback Method
vc	0.894	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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