

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

Inchi:	InChI=1S/C14H18BrNO3/c1-2-3-9-19-13(17)7-8-16-14(18)11-5-4-6-12(15)10-11/h4-6,10
InchiKey:	QZIFJZNLJSXDKN-UHFFFAOYSA-N
Formula:	C14H18BrNO3
SMILES:	CCCCOC(=O)CCNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	328.20

Physical Properties

Property code	Value	Unit	Source
gf	-89.35	kJ/mol	Joback Method
hf	-384.81	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.912		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	797.87	K	Joback Method
tc	1015.73	K	Joback Method
tf	521.03	K	Joback Method
vc	0.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.80	J/mol×K	797.87	Joback Method
cpg	616.38	J/mol×K	834.18	Joback Method
cpg	628.03	J/mol×K	870.49	Joback Method
cpg	638.78	J/mol×K	906.80	Joback Method
cpg	648.68	J/mol×K	943.11	Joback Method
cpg	657.75	J/mol×K	979.42	Joback Method
cpg	666.03	J/mol×K	1015.73	Joback Method

Sources

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=U321640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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