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

Inchi: InChI=1S/C14H18BrNO3/c1-10(2)9-19-13(17)6-7-16-14(18)11-4-3-5-12(15)8-11/h3-5,8,1

InchiKey: JYFXMHPHEMEFFX-UHFFFAOYSA-N

Formula: C14H18BrNO3

SMILES: CC(C)COC(=O)CCNC(=O)c1cccc(Br)c1

Mol. weight [g/mol]: 328.20

Physical Properties

Property code	Value	Unit	Source
gf	-91.79	kJ/mol	Joback Method
hf	-390.09	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.768		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	797.43	K	Joback Method
tc	1018.59	K	Joback Method
tf	506.03	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.39	J/mol×K	797.43	Joback Method
cpg	617.16	J/mol×K	834.29	Joback Method
cpg	628.95	J/mol×K	871.15	Joback Method
cpg	639.81	J/mol×K	908.01	Joback Method
cpg	649.77	J/mol×K	944.87	Joback Method
cpg	658.87	J/mol×K	981.73	Joback Method
cpg	667.15	J/mol×K	1018.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321639&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

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