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

Inchi: InChI=1S/C16H22BrNO3/c1-12(2)5-4-10-21-15(19)8-9-18-16(20)13-6-3-7-14(17)11-13/h

InchiKey: PRJZDHKKNFEHLG-UHFFFAOYSA-N

Formula: C16H22BrNO3

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

Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-74.95	kJ/mol	Joback Method
hf	-431.37	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	82.53	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.548		Crippen Method
mcvol	249.030	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2529.00		NIST Webbook
rinpol	2529.00		NIST Webbook
tb	843.19	K	Joback Method
tc	1060.12	K	Joback Method
tf	528.57	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.40	J/mol×K	843.19	Joback Method
cpg	728.76	J/mol×K	879.34	Joback Method
cpg	741.10	J/mol×K	915.50	Joback Method
cpg	752.48	J/mol×K	951.65	Joback Method
cpg	762.93	J/mol×K	987.81	Joback Method
cpg	772.50	J/mol×K	1023.96	Joback Method
cpg	781.23	J/mol×K	1060.12	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=U321642&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