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

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

InchiKey: XBRSHTBPAALARI-UHFFFAOYSA-N

Formula: C16H22BrNO3

SMILES: CCCCCCOC(=O)CCNC(=O)c1cccc(Br)c1

Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-72.51	kJ/mol	Joback Method
hf	-426.09	kJ/mol	Joback Method
hfus	45.62	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.692		Crippen Method
mcvol	249.030	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	2574.00		NIST Webbook
tb	843.63	K	Joback Method
tc	1057.90	K	Joback Method
tf	543.57	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.83	J/mol×K	843.63	Joback Method
cpg	728.05	J/mol×K	879.34	Joback Method
cpg	740.28	J/mol×K	915.05	Joback Method
cpg	751.59	J/mol×K	950.76	Joback Method
cpg	762.00	J/mol×K	986.48	Joback Method
cpg	771.56	J/mol×K	1022.19	Joback Method
cpg	780.31	J/mol×K	1057.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321643&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