«beta»-Alanine, N-(2-bromobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H26BrNO3/c1-2-3-4-5-6-9-14-23-17(21)12-13-20-18(22)15-10-7-8-11-16(1

InchiKey: FPPGAIQWPXUUIG-UHFFFAOYSA-N

Formula: C18H26BrNO3

SMILES: CCCCCCCCOC(=O)CCNC(=O)c1ccccc1Br

Mol. weight [g/mol]: 384.31

Physical Properties

Property code	Value	Unit	Source
gf	-55.67	kJ/mol	Joback Method
hf	-467.37	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.473		Crippen Method
mcvol	277.210	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	889.39	K	Joback Method
tc	1102.72	K	Joback Method
tf	566.11	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.43	J/mol×K	889.39	Joback Method
cpg	843.18	J/mol×K	924.94	Joback Method
cpg	855.90	J/mol×K	960.50	Joback Method
cpg	867.65	J/mol×K	996.05	Joback Method
cpg	878.47	J/mol×K	1031.61	Joback Method
cpg	888.41	J/mol×K	1067.16	Joback Method
cpg	897.52	J/mol×K	1102.72	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=U321732&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