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

Inchi: InChI=1S/C17H24BrNO3/c1-2-3-4-5-6-12-22-16(20)10-11-19-17(21)14-8-7-9-15(18)13-1

InchiKey: YTWNKSNQMSIDMF-UHFFFAOYSA-N

Formula: C17H24BrNO3

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

Mol. weight [g/mol]: 370.28

Physical Properties

Property code	Value	Unit	Source
gf	-64.09	kJ/mol	Joback Method
hf	-446.73	kJ/mol	Joback Method
hfus	48.21	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.083		Crippen Method
mcvol	263.120	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook
tb	866.51	K	Joback Method
tc	1079.95	K	Joback Method
tf	554.84	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.72	J/mol×K	866.51	Joback Method
cpg	785.21	J/mol×K	902.08	Joback Method
cpg	797.70	J/mol×K	937.66	Joback Method
cpg	809.23	J/mol×K	973.23	Joback Method
cpg	819.86	J/mol×K	1008.81	Joback Method
cpg	829.61	J/mol×K	1044.38	Joback Method
cpg	838.55	J/mol×K	1079.95	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=U321644&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