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

Inchi: InChI=1S/C12H14BrNO3/c1-2-17-11(15)7-8-14-12(16)9-5-3-4-6-10(9)13/h3-6H,2,7-8H2,
InchiKey: ZMKVTXPMZTTWAM-UHFFFAOYSA-N
Formula: C12H14BrNO3
SMILES: CCOC(=O)CCNC(=O)c1ccccc1Br
Mol. weight [g/mol]: 300.15

Physical Properties

Property code	Value	Unit	Source
gf	-106.19	kJ/mol	Joback Method
hf	-343.53	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.132		Crippen Method
mcvol	192.670	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	752.11	K	Joback Method
tc	975.87	K	Joback Method
tf	498.49	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.89	J/mol×K	752.11	Joback Method
cpg	508.65	J/mol×K	789.40	Joback Method
cpg	519.52	J/mol×K	826.70	Joback Method
cpg	529.54	J/mol×K	863.99	Joback Method
cpg	538.74	J/mol×K	901.28	Joback Method
cpg	547.14	J/mol×K	938.57	Joback Method
cpg	554.79	J/mol×K	975.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321727&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