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

Inchi: InChI=1S/C13H16BrNO3/c1-2-8-18-12(16)6-7-15-13(17)10-4-3-5-11(14)9-10/h3-5,9H,2,6

InchiKey: PTJPZNQZNKBUCL-UHFFFAOYSA-N

Formula: C13H16BrNO3

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

Mol. weight [g/mol]: 314.18

Physical Properties

Property code	Value	Unit	Source
gf	-97.77	kJ/mol	Joback Method
hf	-364.17	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	76.24	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.522		Crippen Method
mcvol	206.760	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	774.99	K	Joback Method
tc	995.53	K	Joback Method
tf	509.76	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.80	J/mol×K	774.99	Joback Method
cpg	562.00	J/mol×K	811.75	Joback Method
cpg	573.29	J/mol×K	848.50	Joback Method
cpg	583.70	J/mol×K	885.26	Joback Method
cpg	593.27	J/mol×K	922.02	Joback Method
cpg	602.03	J/mol×K	958.77	Joback Method
cpg	610.02	J/mol×K	995.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321638&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

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