l-Alanine, N-(4-bromobenzoyl)-, methyl ester

Inchi: InChI=1S/C11H12BrNO3/c1-7(11(15)16-2)13-10(14)8-3-5-9(12)6-4-8/h3-7H,1-2H3,(H,13
InchiKey: SMEWLRMRAWWXPJ-UHFFFAOYSA-N
Formula: C11H12BrNO3
SMILES: COC(=O)C(C)NC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 286.12

Physical Properties

Property code	Value	Unit	Source
gf	-117.05	kJ/mol	Joback Method
hf	-328.17	kJ/mol	Joback Method
hfus	29.15	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.740		Crippen Method
mcvol	178.580	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	728.79	K	Joback Method
tc	960.48	K	Joback Method
tf	472.22	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.78	J/mol×K	728.79	Joback Method
cpg	457.24	J/mol×K	767.41	Joback Method
cpg	467.80	J/mol×K	806.02	Joback Method
cpg	477.49	J/mol×K	844.64	Joback Method
cpg	486.34	J/mol×K	883.25	Joback Method
cpg	494.38	J/mol×K	921.87	Joback Method
cpg	501.64	J/mol×K	960.48	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=U299612&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