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

Inchi: InChI=1S/C13H16BrNO3/c1-8(2)11(13(17)18-3)15-12(16)9-4-6-10(14)7-5-9/h4-8,11H,1-3
InchiKey: QXKARJNTOKUFPX-UHFFFAOYSA-N
Formula: C13H16BrNO3
SMILES: COC(=O)C(NC(=O)c1ccc(Br)cc1)C(C)C
Mol. weight [g/mol]: 314.18

Physical Properties

Property code	Value	Unit	Source
gf	-102.65	kJ/mol	Joback Method
hf	-374.73	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.377		Crippen Method
mcvol	206.760	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	2039.00		NIST Webbook
tb	774.11	K	Joback Method
tc	1002.03	K	Joback Method
tf	479.76	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.99	J/mol×K	774.11	Joback Method
cpg	563.60	J/mol×K	812.10	Joback Method
cpg	575.21	J/mol×K	850.08	Joback Method
cpg	585.86	J/mol×K	888.07	Joback Method
cpg	595.59	J/mol×K	926.06	Joback Method
cpg	604.43	J/mol×K	964.05	Joback Method
cpg	612.43	J/mol×K	1002.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299614&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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