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

Inchi: InChI=1S/C14H18BrNO3/c1-9(2)8-12(14(18)19-3)16-13(17)10-4-6-11(15)7-5-10/h4-7,9,1
InchiKey: RIYQPKDTWIBZHR-UHFFFAOYSA-N
Formula: C14H18BrNO3
SMILES: COC(=O)C(CC(C)C)NC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 328.20

Physical Properties

Property code	Value	Unit	Source
gf	-94.23	kJ/mol	Joback Method
hf	-395.37	kJ/mol	Joback Method
hfus	33.39	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.767		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	2116.00		NIST Webbook
tb	796.99	K	Joback Method
tc	1021.61	K	Joback Method
tf	491.03	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.98	J/mol×K	796.99	Joback Method
cpg	617.94	J/mol×K	834.43	Joback Method
cpg	629.89	J/mol×K	871.86	Joback Method
cpg	640.85	J/mol×K	909.30	Joback Method
cpg	650.88	J/mol×K	946.73	Joback Method
cpg	660.01	J/mol×K	984.17	Joback Method
cpg	668.28	J/mol×K	1021.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299615&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