L-Valine, N-(3-bromobenzoyl)-, butyl ester

Inchi: InChI=1S/C16H22BrNO3/c1-4-5-9-21-16(20)14(11(2)3)18-15(19)12-7-6-8-13(17)10-12/h
InchiKey: BGGWBOJSAOUCGG-UHFFFAOYSA-N
Formula: C16H22BrNO3
SMILES: CCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-77.39	kJ/mol	Joback Method
hf	-436.65	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.547		Crippen Method
mcvol	249.030	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	842.75	K	Joback Method
tc	1062.49	K	Joback Method
tf	513.57	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.96	J/mol×K	842.75	Joback Method
cpg	729.48	J/mol×K	879.37	Joback Method
cpg	741.94	J/mol×K	916.00	Joback Method
cpg	753.39	J/mol×K	952.62	Joback Method
cpg	763.89	J/mol×K	989.24	Joback Method
cpg	773.46	J/mol×K	1025.87	Joback Method
cpg	782.17	J/mol×K	1062.49	Joback Method

Sources

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=U346686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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