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

Inchi: InChI=1S/C17H24BrNO3/c1-4-5-6-10-22-17(21)15(12(2)3)19-16(20)13-8-7-9-14(18)11-1
InchiKey: LVROHIZESMZYGZ-UHFFFAOYSA-N
Formula: C17H24BrNO3
SMILES: CCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 370.28

Physical Properties

Property code	Value	Unit	Source
gf	-68.97	kJ/mol	Joback Method
hf	-457.29	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.937		Crippen Method
mcvol	263.120	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	865.63	K	Joback Method
tc	1083.89	K	Joback Method
tf	524.84	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.81	J/mol×K	865.63	Joback Method
cpg	786.55	J/mol×K	902.01	Joback Method
cpg	799.22	J/mol×K	938.38	Joback Method
cpg	810.87	J/mol×K	974.76	Joback Method
cpg	821.55	J/mol×K	1011.13	Joback Method
cpg	831.30	J/mol×K	1047.51	Joback Method
cpg	840.17	J/mol×K	1083.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346687&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