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

Inchi: InChI=1S/C23H36BrNO3/c1-4-5-6-7-8-9-10-11-12-16-28-23(27)21(18(2)3)25-22(26)19-1
InchiKey: QNLMGQYEAWHWHQ-UHFFFAOYSA-N
Formula: C23H36BrNO3
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 454.44

Physical Properties

Property code	Value	Unit	Source
gf	-18.45	kJ/mol	Joback Method
hf	-581.13	kJ/mol	Joback Method
hfus	56.70	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.277		Crippen Method
mcvol	347.660	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
tb	1002.91	K	Joback Method
tc	1228.53	K	Joback Method
tf	592.46	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.15	J/mol×K	1002.91	Joback Method
cpg	1144.18	J/mol×K	1040.51	Joback Method
cpg	1157.98	J/mol×K	1078.12	Joback Method
cpg	1170.60	J/mol×K	1115.72	Joback Method
cpg	1182.13	J/mol×K	1153.32	Joback Method
cpg	1192.65	J/mol×K	1190.93	Joback Method
cpg	1202.21	J/mol×K	1228.53	Joback Method

Sources

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=U346693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume