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

Inchi: InChI=1S/C24H38BrNO3/c1-4-5-6-7-8-9-10-11-12-13-17-29-24(28)22(19(2)3)26-23(27)2
InchiKey: NYXALLIATRMWGO-UHFFFAOYSA-N
Formula: C24H38BrNO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 468.47

Physical Properties

Property code	Value	Unit	Source
gf	-10.03	kJ/mol	Joback Method
hf	-601.77	kJ/mol	Joback Method
hfus	59.29	kJ/mol	Joback Method
hvap	99.95	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	6.668		Crippen Method
mcvol	361.750	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
tb	1025.79	K	Joback Method
tc	1255.86	K	Joback Method
tf	603.73	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.59	J/mol×K	1025.79	Joback Method
cpg	1205.91	J/mol×K	1064.14	Joback Method
cpg	1219.94	J/mol×K	1102.48	Joback Method
cpg	1232.76	J/mol×K	1140.83	Joback Method
cpg	1244.45	J/mol×K	1179.17	Joback Method
cpg	1255.10	J/mol×K	1217.52	Joback Method
cpg	1264.78	J/mol×K	1255.86	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=U346694&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