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

Inchi: InChI=1S/C18H26BrNO3/c1-4-5-6-7-11-23-18(22)16(13(2)3)20-17(21)14-9-8-10-15(19)1
InchiKey: LOXGCZNKWIALOH-UHFFFAOYSA-N
Formula: C18H26BrNO3
SMILES: CCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 384.31

Physical Properties

Property code	Value	Unit	Source
gf	-60.55	kJ/mol	Joback Method
hf	-477.93	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.327		Crippen Method
mcvol	277.210	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	888.51	K	Joback Method
tc	1105.97	K	Joback Method
tf	536.11	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.48	J/mol×K	888.51	Joback Method
cpg	844.43	J/mol×K	924.75	Joback Method
cpg	857.29	J/mol×K	961.00	Joback Method
cpg	869.12	J/mol×K	997.24	Joback Method
cpg	879.95	J/mol×K	1033.49	Joback Method
cpg	889.85	J/mol×K	1069.73	Joback Method
cpg	898.86	J/mol×K	1105.97	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=U346688&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