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

Inchi: InChI=1S/C20H30BrNO3/c1-4-5-6-7-8-9-13-25-20(24)18(15(2)3)22-19(23)16-11-10-12-1
InchiKey: QVDXYLQVRLVOEC-UHFFFAOYSA-N
Formula: C20H30BrNO3
SMILES: CCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 412.36

Physical Properties

Property code	Value	Unit	Source
gf	-43.71	kJ/mol	Joback Method
hf	-519.21	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	91.05	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.107		Crippen Method
mcvol	305.390	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	934.27	K	Joback Method
tc	1152.41	K	Joback Method
tf	558.65	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.05	J/mol×K	934.27	Joback Method
cpg	962.40	J/mol×K	970.63	Joback Method
cpg	975.61	J/mol×K	1006.98	Joback Method
cpg	987.75	J/mol×K	1043.34	Joback Method
cpg	998.86	J/mol×K	1079.70	Joback Method
cpg	1009.01	J/mol×K	1116.06	Joback Method
cpg	1018.26	J/mol×K	1152.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346690&Units=SI

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