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

Inchi: InChI=1S/C15H20BrNO3/c1-4-8-20-15(19)13(10(2)3)17-14(18)11-6-5-7-12(16)9-11/h5-7
InchiKey: KMDJDHUQZNJQIO-UHFFFAOYSA-N
Formula: C15H20BrNO3
SMILES: CCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 342.23

Physical Properties

Property code	Value	Unit	Source
gf	-85.81	kJ/mol	Joback Method
hf	-416.01	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.157		Crippen Method
mcvol	234.940	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	819.87	K	Joback Method
tc	1041.75	K	Joback Method
tf	502.30	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.00	J/mol×K	819.87	Joback Method
cpg	673.25	J/mol×K	856.85	Joback Method
cpg	685.48	J/mol×K	893.83	Joback Method
cpg	696.71	J/mol×K	930.81	Joback Method
cpg	706.99	J/mol×K	967.79	Joback Method
cpg	716.36	J/mol×K	1004.77	Joback Method
cpg	724.87	J/mol×K	1041.75	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=U346685&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