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

Inchi: InChI=1S/C19H28BrNO3/c1-4-5-6-7-8-12-24-19(23)17(14(2)3)21-18(22)15-10-9-11-16(2
InchiKey: FXUXNKPWAXUACQ-UHFFFAOYSA-N
Formula: C19H28BrNO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 398.33

Physical Properties

Property code	Value	Unit	Source
gf	-52.13	kJ/mol	Joback Method
hf	-498.57	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.717		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	911.39	K	Joback Method
tc	1128.80	K	Joback Method
tf	547.38	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.91	J/mol×K	911.39	Joback Method
cpg	903.06	J/mol×K	947.62	Joback Method
cpg	916.10	J/mol×K	983.86	Joback Method
cpg	928.08	J/mol×K	1020.09	Joback Method
cpg	939.06	J/mol×K	1056.33	Joback Method
cpg	949.09	J/mol×K	1092.56	Joback Method
cpg	958.23	J/mol×K	1128.80	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=U346689&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