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

Inchi: InChI=1S/C26H42BrNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-31-26(30)24(21(2)3)28-2
InchiKey: NYHQIRUXKFDJTP-UHFFFAOYSA-N
Formula: C26H42BrNO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C
Mol. weight [g/mol]: 496.52

Physical Properties

Property code	Value	Unit	Source
gf	6.81	kJ/mol	Joback Method
hf	-643.05	kJ/mol	Joback Method
hfus	64.47	kJ/mol	Joback Method
hvap	104.40	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	7.448		Crippen Method
mcvol	389.930	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	3368.00		NIST Webbook
rinpol	3368.00		NIST Webbook
tb	1071.55	K	Joback Method
tc	1313.88	K	Joback Method
tf	626.27	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1314.86	J/mol×K	1071.55	Joback Method
cpg	1330.86	J/mol×K	1111.94	Joback Method
cpg	1345.45	J/mol×K	1152.33	Joback Method
cpg	1358.73	J/mol×K	1192.72	Joback Method
cpg	1370.81	J/mol×K	1233.10	Joback Method
cpg	1381.79	J/mol×K	1273.49	Joback Method
cpg	1391.78	J/mol×K	1313.88	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=U346695&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