L-Valine, N-(2,6-difluorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C24H37F2NO3/c1-4-5-6-7-8-9-10-11-12-13-17-30-24(29)22(18(2)3)27-23(28)2

InchiKey: OCEHRZHSMKNRJC-UHFFFAOYSA-N

Formula: C24H37F2NO3

SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C

Mol. weight [g/mol]: 425.55

Physical Properties

Property code	Value	Unit	Source
gf	-423.60	kJ/mol	Joback Method
hf	-1031.79	kJ/mol	Joback Method
hfus	59.78	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	6.183		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	993.25	kPa	Joback Method
rinpol	2880.00		NIST Webbook
rinpol	2880.00		NIST Webbook
tb	963.15	K	Joback Method
tc	1179.39	K	Joback Method
tf	557.63	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.78	J/mol×K	963.15	Joback Method
cpg	1181.20	J/mol×K	999.19	Joback Method
cpg	1196.25	J/mol×K	1035.23	Joback Method
cpg	1210.00	J/mol×K	1071.27	Joback Method
cpg	1222.49	J/mol×K	1107.31	Joback Method
cpg	1233.78	J/mol×K	1143.35	Joback Method
cpg	1243.93	J/mol×K	1179.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346623&Units=SI
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

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