L-Valine, N-(2,4-difluorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C23H35F2NO3/c1-4-5-6-7-8-9-10-11-12-15-29-23(28)21(17(2)3)26-22(27)19-1

InchiKey: OJCJIMMDSXCLFA-UHFFFAOYSA-N

Formula: C23H35F2NO3

SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1F)C(C)C

Mol. weight [g/mol]: 411.53

Physical Properties

Property code	Value	Unit	Source
gf	-432.02	kJ/mol	Joback Method
hf	-1011.15	kJ/mol	Joback Method
hfus	57.19	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	5.793		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	940.27	K	Joback Method
tc	1151.21	K	Joback Method
tf	546.36	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.41	J/mol×K	940.27	Joback Method
cpg	1119.49	J/mol×K	975.43	Joback Method
cpg	1134.28	J/mol×K	1010.58	Joback Method
cpg	1147.84	J/mol×K	1045.74	Joback Method
cpg	1160.21	J/mol×K	1080.90	Joback Method
cpg	1171.44	J/mol×K	1116.05	Joback Method
cpg	1181.57	J/mol×K	1151.21	Joback Method

Sources

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=U346443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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