L-Valine, N-(2,6-difluoro-3-methylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H37F2NO3/c1-5-6-7-8-9-10-11-12-13-16-30-24(29)22(17(2)3)27-23(28)20-

InchiKey: RQYDGGZPAWCPIY-UHFFFAOYSA-N

Formula: C24H37F2NO3

SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)ccc(C)c1F)C(C)C

Mol. weight [g/mol]: 425.55

Physical Properties

Property code	Value	Unit	Source
gf	-433.23	kJ/mol	Joback Method
hf	-1043.26	kJ/mol	Joback Method
hfus	59.39	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	6.102		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
tb	968.13	K	Joback Method
tc	1185.54	K	Joback Method
tf	570.15	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.09	J/mol×K	968.13	Joback Method
cpg	1180.40	J/mol×K	1004.36	Joback Method
cpg	1195.32	J/mol×K	1040.60	Joback Method
cpg	1208.90	J/mol×K	1076.83	Joback Method
cpg	1221.18	J/mol×K	1113.07	Joback Method
cpg	1232.23	J/mol×K	1149.30	Joback Method
cpg	1242.07	J/mol×K	1185.54	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=U346450&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