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

Inchi: InChI=1S/C25H39F2NO3/c1-5-6-7-8-9-10-11-12-13-14-17-31-25(30)23(18(2)3)28-24(29)

InchiKey: PDAJPCGBRFBHTJ-UHFFFAOYSA-N

Formula: C25H39F2NO3

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

Mol. weight [g/mol]: 439.58

Physical Properties

Property code	Value	Unit	Source
gf	-424.81	kJ/mol	Joback Method
hf	-1063.90	kJ/mol	Joback Method
hfus	61.98	kJ/mol	Joback Method
hvap	95.43	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	6.492		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	991.01	K	Joback Method
tc	1214.86	K	Joback Method
tf	581.42	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.95	J/mol×K	991.01	Joback Method
cpg	1242.61	J/mol×K	1028.32	Joback Method
cpg	1257.79	J/mol×K	1065.63	Joback Method
cpg	1271.54	J/mol×K	1102.94	Joback Method
cpg	1283.91	J/mol×K	1140.25	Joback Method
cpg	1294.96	J/mol×K	1177.56	Joback Method
cpg	1304.75	J/mol×K	1214.86	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=U346451&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