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

Inchi: InChI=1S/C27H43F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-33-27(32)25(21(2)3)3

InchiKey: PVGCDZNJOXCUAI-UHFFFAOYSA-N

Formula: C27H43F2NO3

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

Mol. weight [g/mol]: 467.63

Physical Properties

Property code	Value	Unit	Source
gf	-398.34	kJ/mol	Joback Method
hf	-1093.71	kJ/mol	Joback Method
hfus	67.55	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	7.354		Crippen Method
mcvol	390.060	ml/mol	McGowan Method
pc	834.83	kPa	Joback Method
rinpol	3219.00		NIST Webbook
rinpol	3219.00		NIST Webbook
tb	1031.79	K	Joback Method
tc	1270.65	K	Joback Method
tf	591.44	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.68	J/mol×K	1031.79	Joback Method
cpg	1369.32	J/mol×K	1071.60	Joback Method
cpg	1385.28	J/mol×K	1111.41	Joback Method
cpg	1399.64	J/mol×K	1151.22	Joback Method
cpg	1412.50	J/mol×K	1191.03	Joback Method
cpg	1423.95	J/mol×K	1230.84	Joback Method
cpg	1434.07	J/mol×K	1270.65	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=U346625&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