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

Inchi: InChI=1S/C28H45F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-34-28(33)26(22(2)
InchiKey: KPIQKHCPGBPOFM-UHFFFAOYSA-N
Formula: C28H45F2NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1F)C(C)C
Mol. weight [g/mol]: 481.66

Physical Properties

Property code	Value	Unit	Source
gf	-389.92	kJ/mol	Joback Method
hf	-1114.35	kJ/mol	Joback Method
hfus	70.14	kJ/mol	Joback Method
hvap	101.45	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	7.744		Crippen Method
mcvol	404.150	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
tb	1054.67	K	Joback Method
tc	1303.60	K	Joback Method
tf	602.71	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.76	J/mol×K	1054.67	Joback Method
cpg	1432.89	J/mol×K	1096.16	Joback Method
cpg	1449.20	J/mol×K	1137.65	Joback Method
cpg	1463.80	J/mol×K	1179.13	Joback Method
cpg	1476.78	J/mol×K	1220.62	Joback Method
cpg	1488.26	J/mol×K	1262.11	Joback Method
cpg	1498.35	J/mol×K	1303.60	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=U346447&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