

L-Valine, N-(2,5-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:	OFUBUXUXPQLTGJ-UHFFFAOYSA-N
Formula:	C28H45F2NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)ccc1F)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
mvol	404.150	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook
tb	1054.67	K	Joback Method
tc	1303.60	K	Joback Method
tf	602.71	K	Joback Method
vc	1.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.76	J/molxK	1054.67	Joback Method
cpg	1432.89	J/molxK	1096.16	Joback Method
cpg	1449.20	J/molxK	1137.65	Joback Method
cpg	1463.80	J/molxK	1179.13	Joback Method
cpg	1476.78	J/molxK	1220.62	Joback Method
cpg	1488.26	J/molxK	1262.11	Joback Method
cpg	1498.35	J/molxK	1303.60	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=U346461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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