L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H44F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-36-28(34)25(20(2)3)32-27(33)19-21(29)23(30)24(31)22(35-4)26(19)

InchiKey: DSKJBKZIZSVUIT-UHFFFAOYSA-N

Formula: C28H44F3NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C

Mol. weight [g/mol]: 515.65

Physical Properties

Property code	Value	Unit	Source
gf	-708.99	kJ/mol	Joback Method
hf	-1465.62	kJ/mol	Joback Method
hfus	73.63	kJ/mol	Joback Method
hvap	104.37	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	7.501		Crippen Method
mcvol	411.790	ml/mol	McGowan Method
pc	751.02	kPa	Joback Method
rinpol	3271.00		NIST Webbook
rinpol	3271.00		NIST Webbook
tb	1086.32	K	Joback Method
tc	1355.23	K	Joback Method
tf	650.57	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.81	J/mol×K	1086.32	Joback Method
cpg	1463.53	J/mol×K	1131.14	Joback Method
cpg	1477.81	J/mol×K	1175.96	Joback Method
cpg	1489.71	J/mol×K	1220.77	Joback Method
cpg	1499.32	J/mol×K	1265.59	Joback Method
cpg	1506.71	J/mol×K	1310.41	Joback Method
cpg	1511.97	J/mol×K	1355.23	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=U346439&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