

D-Alanine, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, heptadecyl ester

InChI: InChI=1S/C28H44F3NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-36-28(34)21(2)AVKYYDOHHNJYRN-UHFFFAOYSA-N

Formula: C28H44F3NO4

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

Mol. weight [g/mol]: 515.65

Physical Properties

Property code	Value	Unit	Source
gf	-706.55	kJ/mol	Joback Method
hf	-1460.34	kJ/mol	Joback Method
hfus	77.15	kJ/mol	Joback Method
hvap	104.75	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	7.645		Crippen Method
mcvol	411.790	ml/mol	McGowan Method
pc	747.74	kPa	Joback Method
rinpol	3368.00		NIST Webbook
rinpol	3368.00		NIST Webbook
tb	1086.76	K	Joback Method
tc	1358.92	K	Joback Method
tf	665.57	K	Joback Method
vc	1.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.66	J/molxK	1086.76	Joback Method
cpg	1463.68	J/molxK	1132.12	Joback Method
cpg	1478.21	J/molxK	1177.48	Joback Method
cpg	1490.34	J/molxK	1222.84	Joback Method
cpg	1500.15	J/molxK	1268.20	Joback Method
cpg	1507.71	J/molxK	1313.56	Joback Method
cpg	1513.11	J/molxK	1358.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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