

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

InChI: InChI=1S/C30H48F3NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-38-30(39-40)O1C(=O)C(C)NC(=O)c1cc(F)c(F)c(OC)c1F
InChIKey: LGUGFKMFRARDGM-UHFFFAOYSA-N

Formula: C30H48F3NO4

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

Mol. weight [g/mol]: 543.70

Physical Properties

Property code	Value	Unit	Source
gf	-689.71	kJ/mol	Joback Method
hf	-1501.62	kJ/mol	Joback Method
hfus	82.33	kJ/mol	Joback Method
hvap	109.21	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	8.426		Crippen Method
mvol	439.970	ml/mol	McGowan Method
pc	675.00	kPa	Joback Method
rinpol	3469.00		NIST Webbook
rinpol	3469.00		NIST Webbook
tb	1132.52	K	Joback Method
tc	1436.45	K	Joback Method
tf	688.11	K	Joback Method
vc	1.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.20	J/molxK	1132.52	Joback Method
cpg	1589.96	J/molxK	1183.18	Joback Method
cpg	1604.61	J/molxK	1233.83	Joback Method
cpg	1616.28	J/molxK	1284.49	Joback Method
cpg	1625.10	J/molxK	1335.14	Joback Method
cpg	1631.21	J/molxK	1385.80	Joback Method
cpg	1634.74	J/molxK	1436.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U348454&Units=SI

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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