

Isonipectic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, hexadecyl

InChI:
ester

InChI=1S/C31H45F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-41-29(40)24-18-20-3

InChIKey:

DCDBZYVXFZKVNQ-UHFFFAOYSA-N

Formula:

C31H45F6NO3

SMILES:

CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

593.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.71		Crippen Method
logp	9.601		Crippen Method
mcvol	442.640	ml/mol	McGowan Method
rinpol	3366.00		NIST Webbook
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Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361216&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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