Desipramine, N-pentafluoropropionyl-

Inchi: InChI=1S/C21H21F5N2O/c1-27(19(29)20(22,23)21(24,25)26)13-6-14-28-17-9-4-2-7-15(1
InchiKey: RVVSHGNINMLCRY-UHFFFAOYSA-N
Formula: C21H21F5N2O
SMILES: CN(CCCN1c2ccccc2CCc2ccccc21)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 412.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	4.969		Crippen Method
mcvol	278.750	ml/mol	McGowan Method
rinpol	2475.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374754&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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