Desipramine, N-heptafluorobutyryl-

Inchi: InChI=1S/C22H21F7N2O/c1-30(19(32)20(23,24)21(25,26)22(27,28)29)13-6-14-31-17-9-
InchiKey: MBWOKMXTAMALHG-UHFFFAOYSA-N
Formula: C22H21F7N2O
SMILES: CN(CCCN1c2ccccc2CCc2ccccc21)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 462.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	5.605		Crippen Method
mcvol	296.380	ml/mol	McGowan Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U374755&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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