

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(
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
rinsol	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/ci990307I
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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/54-310-7/Desipramine-N-pentafluoropropionyl.pdf>

Generated by Cheméo on 2024-04-26 05:20:49.703597947 +0000 UTC m=+16398098.624175263.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.