

Desipramine, N-trifluoroacetyl-

Inchi:	InChI=1S/C20H21F3N2O/c1-24(19(26)20(21,22)23)13-6-14-25-17-9-4-2-7-15(17)11-12-
InchiKey:	NWFGPSBXXWZYQB-UHFFFAOYSA-N
Formula:	C20H21F3N2O
SMILES:	CN(CCCN1c2ccccc2CCc2ccccc21)C(=O)C(F)(F)F
Mol. weight [g/mol]:	362.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	4.334		Crippen Method
mcvol	261.120	ml/mol	McGowan Method
rinpola	2506.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374753&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/26-794-2/Desipramine-N-trifluoroacetyl.pdf>

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