Didesmethylimipramine

Inchi:	InChI=1S/C17H20N2/c18-12-5-13-19-16-8-3-1-6-14(16)10-11-15-7-2-4-9-17(15)19/h1-4,(
InchiKey:	XJWJQDZWUYUIEM-UHFFFAOYSA-N
Formula:	C17H20N2
SMILES:	NCCCN1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	252.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.272		Crippen Method
mcvol	211.970	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U298667&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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