

desipramine

Other names:	Pertofran
Inchi:	InChI=1S/C18H22N2/c1-19-13-6-14-20-17-9-4-2-7-15(17)11-12-16-8-3-5-10-18(16)20/h2
InchiKey:	HCYAFALTSJYZDH-UHFFFAOYSA-N
Formula:	C18H22N2
SMILES:	CNCCCN1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	266.38
CAS:	50-47-5

Physical Properties

Property code	Value	Unit	Source
ie	7.39 ± 0.06	eV	NIST Webbook
log10ws	-4.28		Crippen Method
logp	3.533		Crippen Method
mcvol	226.060	ml/mol	McGowan Method
rinpol	2217.00		NIST Webbook
rinpol	2241.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2255.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2242.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C50475&Units=SI>

Legend

ie:	Ionization energy
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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