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]: 266.39

Physical Properties

Property code	Value	Unit	Source
ie	7.39 ± 0.06	eV	NIST Webbook
log10ws	-3.35		Cheméo Relay (1.0)
logp	3.533		Crippen Method
mcvol	226.060	ml/mol	McGowan Method
rinpol	2235.00		NIST Webbook
rinpol	2255.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2241.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tf	384.03	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50475&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tf:	Normal melting (fusion) point