

Desmethyltrimipramine

Other names:	Desmethyltrimipramine
Inchi:	InChI=1S/C19H24N2/c1-15(13-20-2)14-21-18-9-5-3-7-16(18)11-12-17-8-4-6-10-19(17)21
InchiKey:	FUEUKSCRQNPXKS-UHFFFAOYSA-N
Formula:	C19H24N2
SMILES:	CNCC(C)CN1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	280.41

Physical Properties

Property code	Value	Unit	Source
ie	7.03	eV	Cheméo Relay (1.0)
log10ws	-3.72		Cheméo Relay (1.0)
logp	3.779		Crippen Method
mcvol	240.150	ml/mol	McGowan Method
tf	380.38	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2293212&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/82-112-6/Desmethytrimipramine.pdf>

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