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