Imipramine M(HO), acetylated

Inchi: InChI=1S/C21H26N2O2/c1-16(24)25-19-11-12-21-18(15-19)10-9-17-7-4-5-8-20(17)23(21
InchiKey: XQYQDBFQDYVWTQ-UHFFFAOYSA-N
Formula: C21H26N2O2
SMILES: CC(=O)Oc1ccc2c(c1)CCc1ccccc1N2CCCN(C)C
Mol. weight [g/mol]: 338.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	3.800		Crippen Method
mcvol	275.770	ml/mol	McGowan Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook

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=R310922&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.