Dibenzepin M(bis-Nor), acetylated

Inchi: InChI=1S/C18H19N3O2/c1-13(22)19-11-12-21-17-10-6-5-9-16(17)20(2)15-8-4-3-7-14(15
InchiKey: ANVVAWROMUKCMM-UHFFFAOYSA-N
Formula: C18H19N3O2
SMILES: CC(=O)NCCN1C(=O)c2ccccc2N(C)c2ccccc21
Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.551		Crippen Method
mcvol	239.180	ml/mol	McGowan Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310853&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.