Dibenzepin M(Ter-nor), acetylated

Inchi: InChI=1S/C20H21N3O3/c1-14(24)21(3)12-13-22-18-10-6-7-11-19(18)23(15(2)25)17-9-5-
InchiKey: JFWFGWSQPXTHHY-UHFFFAOYSA-N
Formula: C20H21N3O3
SMILES: CC(=O)N(C)CCN1C(=O)c2ccccc2N(C(C)=O)c2ccccc21
Mol. weight [g/mol]: 351.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.810		Crippen Method
mcvol	268.930	ml/mol	McGowan Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310873&Units=SI
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

Legend

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

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