Perazine M (nor-), monoacetylated

Inchi: InChI=1S/C21H25N3OS/c1-17(25)23-15-13-22(14-16-23)11-6-12-24-18-7-2-4-9-20(18)2
InchiKey: RKTFUOCNNWAYFW-UHFFFAOYSA-N
Formula: C21H25N3OS
SMILES: CC(=O)N1CCN(CCCN2c3ccccc3Sc3ccccc32)CC1
Mol. weight [g/mol]: 367.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.844		Crippen Method
mcvol	285.370	ml/mol	McGowan Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310477&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

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