

Pecazine M (HO-), monoacetylated

Inchi: InChI=1S/C21H24N2O2S/c1-15(24)25-17-9-10-19-21(12-17)26-20-8-4-3-7-18(20)23(19)
InchiKey: CJFTUQHGGQYCMGK-UHFFFAOYSA-N
Formula: C21H24N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC1CCCN(C)C1
Mol. weight [g/mol]: 368.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.556		Crippen Method
mcvol	281.260	ml/mol	McGowan Method
rinpol	2750.00		NIST Webbook

Sources

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=R310437&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/39-924-3/Pecazine-M-HO-monoacetylated.pdf>

Generated by Cheméo on 2024-04-23 07:24:43.10292893 +0000 UTC m=+16146332.023506252.

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