

Dixyrazine, monoacetylated

Inchi: InChI=1S/C26H35N3O3S/c1-21(19-28-13-11-27(12-14-28)15-16-31-17-18-32-22(2)30)2
InchiKey: LAHKSILSJFAQLI-UHFFFAOYSA-N
Formula: C26H35N3O3S
SMILES: CC(=O)OCCOCCN1CCN(CC(C)CN2c3ccccc3Sc3ccccc32)CC1
Mol. weight [g/mol]: 469.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	4.123		Crippen Method
mcvol	367.560	ml/mol	McGowan Method
rinpol	3531.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R310308&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

Latest version available from:

<https://www.chemeo.com/cid/17-072-3/Dixyrazine-monoacetylated.pdf>

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