Dixyrazine M (O-desalkyl-), monoacetylated

Inchi: InChI=1S/C24H31N3O2S/c1-19(17-26-13-11-25(12-14-26)15-16-29-20(2)28)18-27-21-7-
InchiKey: JMKZUSPFNSRQHY-UHFFFAOYSA-N
Formula: C24H31N3O2S
SMILES: CC(=O)OCCN1CCN(CC(C)CN2c3ccccc3Sc3ccccc32)CC1
Mol. weight [g/mol]: 425.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	4.106		Crippen Method
mcvol	333.510	ml/mol	McGowan Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310299&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

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