Clopenthixol, monoacetylated

Inchi: InChI=1S/C24H27ClN2O2S/c1-18(28)29-16-15-27-13-11-26(12-14-27)10-4-6-20-21-5-2-
InchiKey: OXAUOBQMCDIVPQ-CGOBSMCZSA-N
Formula: C24H27ClN2O2S
SMILES: CC(=O)OCCN1CCN(CCC=C2c3ccccc3Sc3ccc(Cl)cc32)CC1
Mol. weight [g/mol]: 443.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	4.807		Crippen Method
mcvol	331.470	ml/mol	McGowan Method
rinpol	3462.00		NIST Webbook
rinpol	3462.00		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=R310259&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.