

Trazodone M(HO), acetylated

Inchi: InChI=1S/C21H24ClN5O3/c1-16(28)30-19-7-6-17(15-18(19)22)25-13-11-24(12-14-25)8-4
InchiKey: GWYAWMGTBHKZSP-UHFFFAOYSA-N
Formula: C21H24ClN5O3
SMILES: CC(=O)Oc1ccc(N2CCN(CCCn3nc4ccccn4c3=O)CC2)cc1Cl
Mol. weight [g/mol]: 429.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	2.287		Crippen Method
mcvol	308.660	ml/mol	McGowan Method
rinsol	3380.00		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=R311227&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/53-845-5/Trazodone-M-HO-acetylated.pdf>

Generated by Cheméo on 2024-04-28 22:12:01.954053769 +0000 UTC m=+16631570.874631084.

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