Oxatomide M (carbinol), acetylated

Inchi: InChI=1S/C12H14N2O3/c1-9(15)17-8-4-7-14-11-6-3-2-5-10(11)13-12(14)16/h2-3,5-6H,4
InchiKey: UUYJFWDEEDGSIU-UHFFFAOYSA-N
Formula: C12H14N2O3
SMILES: CC(=O)OCCCn1c(=O)[nH]c2ccccc21
Mol. weight [g/mol]: 234.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	0.801		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		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=R536659&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.