7,8,9,10-Tetrahydro-6H-cyclohepta[d]pyrido[1,2-a]

Inchi: InChI=1S/C14H22N2O/c1-10-6-5-9-16-13(10)15-12-8-4-2-3-7-11(12)14(16)17/h10-12H,2
InchiKey: OZUSAQQZGMQBQX-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: CC1CCCN2C(=O)C3CCCCCC3N=C12
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	2.606		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
rinpol	2158.00		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=R318406&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