

4H,6h-m-dioxino[4',5':5,6]pyrano[4,3-d]-4-oxazolin-2-one-hexahydro-4-methoxy-1,8-diphenyl-

InChI: InChI=1S/C21H21NO6/c1-24-20-18-15(22(21(23)28-18)14-10-6-3-7-11-14)17-15(26-20)
InChIKey: JRYKXBWNMFZUBT-UHFFFAOYSA-N

Formula: C₂₁H₂₁NO₆
SMILES: COC1OC2COC(c3ccccc3)OC2C2C1OC(=O)N2c1ccccc1
Mol. weight [g/mol]: 383.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.866		Crippen Method
mcvol	267.550	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008323&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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