

Metergoline

Inchi: InChI=1S/C25H29N3O2/c1-27-14-18(13-26-25(29)30-16-17-7-4-3-5-8-17)11-21-20-9-6-1
InchiKey: WZHJKEUHNJHDLS-FBHNJWQJSA-N
Formula: C25H29N3O2
SMILES: CN1CC(CNC(=O)OCc2ccccc2)CC2c3cccc4c3c(cn4C)CC21
Mol. weight [g/mol]: 403.52
CAS: 17692-51-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.01		Crippen Method
logp	4.065		Crippen Method
mcvol	316.090	ml/mol	McGowan Method
rinpol	2741.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17692512&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/54-781-5/Metergoline.pdf>

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