3H-Pyrimidin-4-one, 2,3:5,6-bis-trimethyleno

Other names: 1,2,3,5,6,7-Hexahydro-3a,8-diaza-s-indacen-4-one
Inchi: InChI=1S/C10H12N2O/c13-10-7-3-1-4-8(7)11-9-5-2-6-12(9)10/h1-6H2
InchiKey: BRFWYALXFLAMPV-UHFFFAOYSA-N
Formula: C10H12N2O
SMILES: O=c1c2c(nc3n1CCC3)CCC2
Mol. weight [g/mol]: 176.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	0.678		Crippen Method
mcvol	132.110	ml/mol	McGowan Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119754&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

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