4H-Cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-o 6,7,8,9-tetrahydro, 7-methyl

Inchi:	InChI=1S/C12H12N2O/c1-8-2-3-9-6-11-13-5-4-12(15)14(11)7-10(8)9/h4-8H,2-3H2,1H3
InchiKey:	ZXAVUBKRVYIVSX-UHFFFAOYSA-N
Formula:	C12H12N2O
SMILES:	CC1CCc2cc3nccc(=O)n3cc21
Mol. weight [g/mol]:	200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.744		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	1998.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R64215&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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