

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

Inchi:	InChI=1S/C16H24N2O/c19-16-13-9-5-1-2-6-10-14(13)17-15-11-7-3-4-8-12-18(15)16/h1-
InchiKey:	HDLNWUHGJLAWLE-UHFFFAOYSA-N
Formula:	C16H24N2O
SMILES:	O=c1c2c(nc3n1CCCCC3)CCCCC2
Mol. weight [g/mol]:	260.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.019		Crippen Method
mcvol	216.650	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R119749&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
rinpol:	Non-polar retention indices

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