

Cyclohexanol, 2-(9h-purin-9-yl)-, trans-

Inchi:	InChI=1S/C11H14N4O/c16-10-4-2-1-3-9(10)15-7-14-8-5-12-6-13-11(8)15/h5-7,9-10,16H
InchiKey:	VJLPIPHTBGYWGJ-UHFFFAOYSA-N
Formula:	C11H14N4O
SMILES:	OC1CCCCC1n1cnc2cncnc21
Mol. weight [g/mol]:	218.26
CAS:	100057-61-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	1.302		Crippen Method
mcvol	161.860	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100057612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/83-493-3/Cyclohexanol-2-9h-purin-9-yl-trans.pdf>

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