

1-Methyl-9-[(1e)-1-propenyl]-1,9-dihydro-6h-purin-

Inchi:	InChI=1S/C9H10N4O/c1-3-4-13-6-10-7-8(13)11-5-12(2)9(7)14/h3-6H,1-2H3/b4-3+
InchiKey:	GUROFOVTNBUSTG-ONEGZZNKSA-N
Formula:	C9H10N4O
SMILES:	CC=Cn1cnc2c(=O)n(C)cnc21
Mol. weight [g/mol]:	190.20
CAS:	4121-44-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	0.621		Crippen Method
mcvol	140.240	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=C4121442&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

Latest version available from:

<https://www.chemeo.com/cid/41-554-1/1-Methyl-9-1e-1-propenyl-1-9-dihydro-6h-purin-6-one.pdf>

Generated by Cheméo on 2024-04-27 03:45:01.504185715 +0000 UTC m=+16478750.424763031.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.