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/ci990307l
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