Purine-8-methanol

Inchi: InChI=1S/C6H6N4O/c11-2-5-9-4-1-7-3-8-6(4)10-5/h1,3,11H,2H2,(H,7,8,9,10)
InchiKey: NFZTXJKXCFQRGN-UHFFFAOYSA-N
Formula: C6H6N4O
SMILES: OCc1nc2cncnc2[nH]1
Mol. weight [g/mol]: 150.14
CAS: 6642-26-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	-0.637		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6642268&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