

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

Latest version available from:

<https://www.chemeo.com/cid/96-900-6/Purine-8-methanol.pdf>

Generated by Cheméo on 2025-12-19 15:56:42.728279638 +0000 UTC m=+5908000.258320293.

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