

Purine, 2,6-bis(methylamino)-

Inchi:	InChI=1S/C7H10N6/c1-8-5-4-6(11-3-10-4)13-7(9-2)12-5/h3H,1-2H3,(H3,8,9,10,11,12,13)
InchiKey:	UOAILLAMPSSARV-UHFFFAOYSA-N
Formula:	C7H10N6
SMILES:	CNc1nc(NC)c2[nH]cnc2n1
Mol. weight [g/mol]:	178.19
CAS:	6333-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	-0.046		Crippen Method
mcvol	130.450	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6333660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/37-757-1/Purine-2-6-bis-methylamino.pdf>

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