

9H-purine-6(1h)-one, 2-amino-9-ethyl-

Inchi:	InChI=1S/C7H9N5O/c1-2-12-3-9-4-5(12)10-7(8)11-6(4)13/h3H,2H2,1H3,(H3,8,10,11,13)
InchiKey:	WDOYBEPLTCFIRQ-UHFFFAOYSA-N
Formula:	C7H9N5O
SMILES:	CCn1cnc2c(=O)[nH]c(N)nc21
Mol. weight [g/mol]:	179.18
CAS:	879-08-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	-0.760		Crippen Method
mcvol	126.340	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C879083&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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