

9H-purin-6(1h)-one, 9-ethyl-

Inchi:	InChI=1S/C7H8N4O/c1-2-11-4-10-5-6(11)8-3-9-7(5)12/h3-4H,2H2,1H3,(H,8,9,12)
InchiKey:	COBZZWPZKRRPEN-UHFFFAOYSA-N
Formula:	C7H8N4O
SMILES:	CCn1cnc2c(=O)[nH]cnc21
Mol. weight [g/mol]:	164.16
CAS:	31010-51-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	-0.342		Crippen Method
mcvol	116.360	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=C31010512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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