

Pyruvic acid, 9h-purin-6-yl-hydrazone

Inchi:	InChI=1S/C8H8N6O2/c1-4(8(15)16)13-14-7-5-6(10-2-9-5)11-3-12-7/h2-3H,1H3,(H,15,16)
InchiKey:	BFLXMTBMGLYBSY-UHFFFAOYSA-N
Formula:	C8H8N6O2
SMILES:	CC(=NNc1ncnc2[nH]cnc12)C(=O)O
Mol. weight [g/mol]:	220.19
CAS:	6642-25-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	-0.257		Crippen Method
mcvol	147.680	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=C6642257&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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