

Nicotinaldehyde, 6-purinyldiazone

Inchi:	InChI=1S/C11H9N7/c1-2-8(4-12-3-1)5-17-18-11-9-10(14-6-13-9)15-7-16-11/h1-7H,(H2,1
InchiKey:	OYHLLLEIHNUZMHX-YAXRCOADSA-N
Formula:	C11H9N7
SMILES:	C(=NNc1ncnc2nc[nH]c12)c1cccnc1
Mol. weight [g/mol]:	239.24
CAS:	6298-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	0.712		Crippen Method
mvol	168.730	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=C6298164&Units=SI

Legend

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

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