

Benzaldehyde, p-nitro-, purin-6-yl-hydrazone

Inchi:	InChI=1S/C12H9N7O2/c20-19(21)9-3-1-8(2-4-9)5-17-18-12-10-11(14-6-13-10)15-7-16-1
InchiKey:	VCVLJCHFJSSSEDG-YAXRCOADSA-N
Formula:	C12H9N7O2
SMILES:	O=[N+](O)c1ccc(C=NNc2ncnc3nc[nH]c23)cc1
Mol. weight [g/mol]:	283.25
CAS:	6331-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	1.225		Crippen Method
mcvol	190.260	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=C6331039&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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