

Inosine, 2'-deoxy-

Other names:	Deoxyinosine Hypoxanthine, 9-(2-deoxy-«beta»-D-erythro-pentofuranosyl)- 2'-Deoxyinosine
Inchi:	InChI=1S/C10H12N4O4/c15-2-6-5(16)1-7(18-6)14-4-13-8-9(14)11-3-12-10(8)17/h3-7,15
InchiKey:	VGONTNSXDCQUGY-UHFFFAOYSA-N
Formula:	C10H12N4O4
SMILES:	OCC1OC(n2cnc3c(O)ncnc32)CC1O
Mol. weight [g/mol]:	252.23
CAS:	890-38-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	-0.827		Crippen Method
mcvol	165.380	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=C890380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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<https://www.chemeo.com/cid/122-817-9/Inosine-2-deoxy.pdf>

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