

Xanthine, 7-(5'-oxohexyl)-3-methyl-1-propyl

Inchi:	InChI=1S/C15H22N4O3/c1-4-8-18-13-12(17(3)10-16-13)14(21)19(15(18)22)9-6-5-7-11(2)
InchiKey:	OBBUXRYSLGAAGJ-UHFFFAOYSA-N
Formula:	C15H22N4O3
SMILES:	CCCN1c(=O)n(CCCCC(C)=O)c(=O)c2c1ncn2C
Mol. weight [g/mol]:	306.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	1.066		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook

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=R146157&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/83-532-9/Xanthine-7-5-oxohexyl-3-methyl-1-propyl.pdf>

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