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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R146157&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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