

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

Inchi: InChI=1S/C15H24N4O3/c1-4-8-18-13-12(17(3)10-16-13)14(21)19(15(18)22)9-6-5-7-11(2)
InchiKey: CFWGPJYVEQHOKP-UHFFFAOYSA-N
Formula: C15H24N4O3
SMILES: CCCn1c(=O)n(CCCCC(C)O)c(=O)c2c1ncn2C
Mol. weight [g/mol]: 308.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	0.858		Crippen Method
mcvol	240.820	ml/mol	McGowan Method
rinpol	2575.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R146122&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

Latest version available from:

<https://www.chemeo.com/cid/60-931-1/Xanthine-1-5-hydroxyhexyl-3-methyl-7-propyl.pdf>

Generated by Cheméo on 2025-12-20 03:58:25.920146813 +0000 UTC m=+5951303.450187467.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.