1-(6'-oxoheptyl)-3,7-dimethylxanthine

Inchi: InChI=1S/C14H20N4O3/c1-10(19)7-5-4-6-8-18-13(20)11-12(15-9-16(11)2)17(3)14(18)21
InchiKey: AFYDQCTVFDKATD-UHFFFAOYSA-N
Formula: C14H20N4O3
SMILES: CC(=O)CCCCCn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.10		Crippen Method
logp	0.583		Crippen Method
mcvol	222.430	ml/mol	McGowan Method
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R155072&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
rinpol: Non-polar retention indices

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