Paraxanthine, n-propyl derivative

Inchi: InChI=1S/C10H14N4O2/c1-4-5-14-8-7(12(2)6-11-8)9(15)13(3)10(14)16/h6H,4-5H2,1-3H
InchiKey: DHYGGYFMXYRIGJ-UHFFFAOYSA-N
Formula: C10H14N4O2
SMILES: CCCn1c(=O)n(C)c(=O)c2c1ncn2C
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	-0.156		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
rinpol	1999.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R270938&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