Theobromine, n-propyl derivative

Inchi: InChI=1S/C10H14N4O2/c1-4-5-14-9(15)7-8(11-6-12(7)2)13(3)10(14)16/h6H,4-5H2,1-3H
InchiKey: XJKSERUTELYNMR-UHFFFAOYSA-N
Formula: C10H14N4O2
SMILES: CCCn1c(=O)c2c(ncn2C)n(C)c1=O
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	1996.00		NIST Webbook
rinpol	1996.00		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=R270943&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

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