7-Methylxanthine

Inchi: InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
InchiKey: PFWLFWPASULGAN-UHFFFAOYSA-N
Formula: C6H6N4O2
SMILES: Cn1cnc2[nH]c(=O)[nH]c(=O)c21
Mol. weight [g/mol]: 166.14

Physical Properties

Property code	Value	Unit	Source
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-1.96		Cheméo Relay (1.0)
logp	-2.014		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
tf	630.29	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C552625

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point