

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

Latest version available from:

<https://www.cheméo.com/cid/102-220-3/7-Methylxanthine.pdf>

Generated by Cheméo on 2026-07-21 16:53:17.488223569 +0000 UTC m=+163893.330108987.

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