9-METHYLPOXANTHINE

Other names: 9-Methylhypoxanthine
Inchi: InChI=1S/C6H6N4O/c1-10-3-9-4-5(10)7-2-8-6(4)11/h2-3H,1H3,(H,7,8,11)
InchiKey: PESGUQRDJASXOR-UHFFFAOYSA-N
Formula: C6H6N4O
SMILES: Cn1cnc2c(=O)[nH]cnc21
Mol. weight [g/mol]: 150.14

Physical Properties

Property code	Value	Unit	Source
hsub	84.00	kJ/mol	NIST Webbook
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-1.26		Cheméo Relay (1.0)
logp	-0.825		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
tf	563.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	84.00	kJ/mol	526.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C875310&Units=SI
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):

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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