Guanine, 1,9-dimethyl-

Inchi: InChI=1S/C7H9N5O/c1-11-3-9-4-5(11)10-7(8)12(2)6(4)13/h3H,1-2H3,(H2,8,10)
InchiKey: MXLVASHNANBJDZ-UHFFFAOYSA-N
Formula: C7H9N5O
SMILES: Cn1c(N)nc2c(ncn2C)c1=O
Mol. weight [g/mol]: 179.18
CAS: 42484-34-4

Physical Properties

Property code	Value	Unit	Source
ie	8.09	eV	NIST Webbook
log10ws	-4.44		Crippen Method
logp	-0.751		Crippen Method
mcvol	126.340	ml/mol	McGowan Method

Sources

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=C42484344&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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