2(1H)Pyrimidinone,4-(dimethylamino)-1-methyl-

Inchi: InChI=1S/C7H11N3O/c1-9(2)6-4-5-10(3)7(11)8-6/h4-5H,1-3H3
InchiKey: DHGBSOMRGXWRSE-UHFFFAOYSA-N
Formula: C7H11N3O
SMILES: CN(C)c1ccn(C)c(=O)n1
Mol. weight [g/mol]: 153.18
CAS: 2228-27-5

Physical Properties

Property code	Value	Unit	Source
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	-0.154		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2228275&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices