

2,4-Diazidopyrimidine

Inchi: InChI=1S/C4H2N8/c5-11-9-3-1-2-7-4(8-3)10-12-6/h1-2H
InchiKey: MIMQLFWRQOEHW-UHFFFAOYSA-N
Formula: C4H2N8
SMILES: [N-]=[N+]=Nc1ccnc(N=[N+]=[N-])n1
Mol. weight [g/mol]: 162.11
CAS: 81686-10-4

Physical Properties

Property code	Value	Unit	Source
chs	-2564.00	kJ/mol	NIST Webbook
log10ws	-12.31		Crippen Method
logp	2.360		Crippen Method
mcvol	106.100	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C81686104&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/77-687-5/2-4-Diazidopyrimidine.pdf>

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