2,4-Diazido-6-methylpyrimidine

Inchi: InChI=1S/C5H4N8/c1-3-2-4(10-12-6)9-5(8-3)11-13-7/h2H,1H3
InchiKey: DHJBZPFQYMVUGZ-UHFFFAOYSA-N
Formula: C5H4N8
SMILES: Cc1cc(N=[N+]=[N-])nc(N=[N+]=[N-])n1
Mol. weight [g/mol]: 176.14
CAS: 1680-11-1

Physical Properties

Property code	Value	Unit	Source
chs	-2818.00	kJ/mol	NIST Webbook
log10ws	-12.79		Crippen Method
logp	2.669		Crippen Method
mcvol	120.190	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=C1680111&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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