2,3-Diazabicyclo[2.2.2]octa-2,5-diene N-oxide

Inchi: InChI=1S/C6H8N2O/c9-8-6-3-1-5(7-8)2-4-6/h1,3,5-6H,2,4H2
InchiKey: REZPTDSIISBQTI-UHFFFAOYSA-N
Formula: C6H8N2O
SMILES: [O-][N+]1=NC2C=CC1CC2
Mol. weight [g/mol]: 124.14
CAS: 37436-17-2

Physical Properties

Property code	Value	Unit	Source
hf	221.00 ± 2.10	kJ/mol	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.050		Crippen Method
mcvol	90.910	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=C37436172&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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