6,7-Diazatricyclo[3.2.2.0(2,4)]non-6-ene, oxide

Inchi: InChI=1S/C7H10N2O/c10-9-7-2-1-6(8-9)4-3-5(4)7/h4-7H,1-3H2
InchiKey: IGSXSBMSJKIJIH-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: [O-][N+]1=NC2CCC1C1CC21
Mol. weight [g/mol]: 138.17
CAS: 25926-99-2

Physical Properties

Property code	Value	Unit	Source
hf	226.10 ± 1.90	kJ/mol	NIST Webbook
log10ws	-1.33		Crippen Method
logp	1.130		Crippen Method
mcvol	98.440	ml/mol	McGowan Method
tf	411.40 ± 1.00	K	NIST Webbook

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=C25926992&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
tf: Normal melting (fusion) point

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