BENZO[B]-1,4-DIAZABICYCLO[2.2.2]OCTENE

Other names: Benzo[b]-1,4-diazabicyclo[2.2.2]octane
Inchi: InChI=1S/C10H12N2/c1-2-4-10-9(3-1)11-5-7-12(10)8-6-11/h1-4H,5-8H2
InchiKey: OGEXWIXITOCNRZ-UHFFFAOYSA-N
Formula: C10H12N2
SMILES: c1ccc2c(c1)N1CCN2CC1
Mol. weight [g/mol]: 160.22

Physical Properties

Property code	Value	Unit	Source
ie	7.92	eV	NIST Webbook
logp	1.327		Crippen Method
mcvol	126.240	ml/mol	McGowan Method
tf	437.52	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7140456&Units=SI

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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