1-BENZOYLIMIDAZOLE

Other names: 1-Benzoylimidazole
1H-Imidazole, 1-benzoyl-
Inchi: InChI=1S/C10H8N2O/c13-10(12-7-6-11-8-12)9-4-2-1-3-5-9/h1-8H
InchiKey: JEGIFBGJZPYMJS-UHFFFAOYSA-N
Formula: C10H8N2O
SMILES: O=C(c1ccccc1)n1ccnc1
Mol. weight [g/mol]: 172.19

Physical Properties

Property code	Value	Unit	Source
hvap	88.71	kJ/mol	Cheméo Relay (1.0)
ie	9.29	eV	Cheméo Relay (1.0)
logp	1.572		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
tb	597.35	K	Cheméo Relay (1.0)
tf	359.55	K	Cheméo Relay (1.0)

Sources

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=C10364940&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point