

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

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