N-Phenylisatin

Other names:	1H-Indole-2,3-dione, 1-phenyl-
	1-Phenyl-indole-2,3-dione
	1-Phenylisatin
	N-Phenylisatin
Inchi:	InChI=1S/C14H9NO2/c16-13-11-8-4-5-9-12(11)15(14(13)17)10-6-2-1-3-7-10/h1-9H
InchiKey:	UWCPWBIMRYXUOU-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=C1C(=O)N(c2ccccc2)c2ccccc21
Mol. weight [g/mol]:	223.23

Physical Properties

Property code	Value	Unit	Source
ie	8.14	eV	Cheméo Relay (1.0)
logp	2.548		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
tf	450.44	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=C723897&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point