

1H-Indene-1,3(2H)-dione, 2-(2-pyridinyl)-

Other names:	1,3-Indandione, 2-(2-pyridyl)- Pyrophthalone 2-(1,3-Dioxohydrindenyl-(2))pyridine 2-(2-Pyridyl)-1,3-indandione 2-(2'-Pyridyl)-indan-1,3-dione
Inchi:	InChI=1S/C14H9NO2/c16-13-9-5-1-2-6-10(9)14(17)12(13)11-7-3-4-8-15-11/h1-8,12H
InchiKey:	CFFKWZMLWPANQE-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=C1c2ccccc2C(=O)C1c1cccn1
Mol. weight [g/mol]:	223.23
CAS:	641-63-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.244		Crippen Method
mcvol	162.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C641634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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