1(2H)-Isoquinolinone, 2-methyl-

Inchi: InChI=1S/C10H9NO/c1-11-7-6-8-4-2-3-5-9(8)10(11)12/h2-7H,1H3
InchiKey: YJRMHIKEMDTYDR-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: Cn1ccc2ccccc2c1=O
Mol. weight [g/mol]: 159.18
CAS: 4594-71-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	1.538		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
tf	328.90 ± 1.00	K	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4594712&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.