

3H-Indazol-3-one, 1,2-dihydro-

Other names:	3-Indazolinone Indazolinone 1H-Indazol-3-ol 3-Hydroxy-1H-indazole 3-Oxo-1,2-indazole 1,2-Dihydro-3H-indazol-3-one 2,3-Dihydro-1H-indazol-3-one 1,2-Dihydroindazol-3-one NSC 9352
Inchi:	InChI=1S/C7H6N2O/c10-7-5-3-1-2-4-6(5)8-9-7/h1-4H,(H2,8,9,10)
InchiKey:	SWEICGMKXPNXNU-UHFFFAOYSA-N
Formula:	C7H6N2O
SMILES:	O=c1[nH][nH]c2ccccc12
Mol. weight [g/mol]:	134.14
CAS:	7364-25-2

Physical Properties

Property code	Value	Unit	Source
hsub	127.60 ± 1.50	kJ/mol	NIST Webbook
log10ws	-1.14		Crippen Method
logp	-0.108		Crippen Method
mcvol	96.400	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7364252&Units=SI

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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