

# Isatoic anhydride

<b>Other names:</b>	Isato acid anhydride 2H-3,1-Benzoxazine-2,4(1H)-dione Anthranilic acid, N-carboxy-, cyclic anhydride Benzoic acid, 2-(carboxyamino)-, cyclic anhydride Isatoic acid anhydride IA 4H-3,1-benzoxazine-2,4(1H)-dione
<b>Inchi:</b>	InChI=1S/C8H5NO3/c10-7-5-3-1-2-4-6(5)9-8(11)12-7/h1-4H,(H,9,11)
<b>InchiKey:</b>	TXJUTRJFNRYTHH-UHFFFAOYSA-N
<b>Formula:</b>	C8H5NO3
<b>SMILES:</b>	O=c1[nH]c2ccccc2c(=O)o1
<b>Mol. weight [g/mol]:</b>	163.13
<b>CAS:</b>	118-48-9

## Physical Properties

Property code	Value	Unit	Source
hsub	115.60 ± 2.80	kJ/mol	NIST Webbook
hsub	82.70 ± 2.80	kJ/mol	NIST Webbook
log10ws	-5.07		Crippen Method
logp	-6.000e-04		Crippen Method
mvol	107.950	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C118489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C118489&amp;Units=SI</a>

## 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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