

# 2H-Isoindole-2-propanoic acid, 1,3-dihydro-1,3-dioxo-

<b>Other names:</b>	Phthalyl-«beta»-alanine 3-Phthalimidopropionic acid 1,3-dihydro-1,3-dioxo-2H-isoindole-2-propionic acid
<b>Inchi:</b>	InChI=1S/C11H9NO4/c13-9(14)5-6-12-10(15)7-3-1-2-4-8(7)11(12)16/h1-4H,5-6H2,(H,13
<b>InchiKey:</b>	DXXHRZUOTPMGEH-UHFFFAOYSA-N
<b>Formula:</b>	C11H9NO4
<b>SMILES:</b>	O=C(O)CCN1C(=O)c2ccccc2C1=O
<b>Mol. weight [g/mol]:</b>	219.19
<b>CAS:</b>	3339-73-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	0.757		Crippen Method
mcvol	151.790	ml/mol	McGowan Method

## Sources

<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=C3339739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3339739&amp;Units=SI</a>
<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>

## Legend

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

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