

# 1H-Pyrrole-2,5-dione, 1-ethyl-

<b>Other names:</b>	Maleimide, N-ethyl- Ethylmaleimide Maleic acid N-ethylimide N-Ethylmaleimide NEM USAF B-121
<b>Inchi:</b>	InChI=1S/C6H7NO2/c1-2-7-5(8)3-4-6(7)9/h3-4H,2H2,1H3
<b>InchiKey:</b>	HDFGOPSGAURCEO-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO2
<b>SMILES:</b>	CCN1C(=O)C=CC1=O
<b>Mol. weight [g/mol]:</b>	125.13
<b>CAS:</b>	128-53-0

## Physical Properties

Property code	Value	Unit	Source
ea	1.12 ± 0.09	eV	NIST Webbook
log10ws	-0.20		Crippen Method
logp	-0.069		Crippen Method
mvol	93.360	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=C128530&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128530&amp;Units=SI</a>

## Legend

<b>ea:</b>	Electron affinity
<b>log10ws:</b>	Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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