

# 1,4-Dioxo-1,2,3,4-tetrahydrophthalazine

<b>Other names:</b>	Phthalhydrazide 1,4-Phthalazinedione, 2,3-dihydro- Phthalazine-1,4-dione Phthalazine-1,4(2H,3H)-dione 2,3-dihydrophthalazine-1,4-dione
<b>Inchi:</b>	InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)8(12)10-9-7/h1-4H,(H,9,11)(H,10,12)
<b>InchiKey:</b>	KGLPWQKSKUVKMJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O2
<b>SMILES:</b>	O=c1[nH][nH]c(=O)c2ccccc12
<b>Mol. weight [g/mol]:</b>	138.12
<b>CAS:</b>	1445-69-8

## Physical Properties

Property code	Value	Unit	Source
hsub	139.80 ± 0.70	kJ/mol	NIST Webbook
log10ws	-0.56		Crippen Method
logp	-0.747		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	132.70 ± 0.70	kJ/mol	439.00	NIST Webbook

## Sources

<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=C1445698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1445698&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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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