

# 2H-1-Benzopyran-2-one, 7-(diethylamino)-

<b>Other names:</b>	Coumarine, 7-diethylamino- Coumarin, 7-diethylamino- 7-(diethylamino)-2-benzopyrone
<b>Inchi:</b>	InChI=1S/C13H15NO2/c1-3-14(4-2)11-7-5-10-6-8-13(15)16-12(10)9-11/h5-9H,3-4H2,1-2
<b>InchiKey:</b>	QXAMGWKESXGGNV-UHFFFAOYSA-N
<b>Formula:</b>	C13H15NO2
<b>SMILES:</b>	CCN(CC)c1ccc2ccc(=O)oc2c1
<b>Mol. weight [g/mol]:</b>	217.26
<b>CAS:</b>	20571-42-0

## Physical Properties

Property code	Value	Unit	Source
ie	7.41	eV	NIST Webbook
log10ws	-7.18		Crippen Method
logp	2.639		Crippen Method
mcvol	172.530	ml/mol	McGowan Method

## 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=C20571420&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20571420&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>ie:</b>	Ionization energy
<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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