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

Other names:	Coumarine, 7-diethylamino- Coumarin, 7-diethylamino- 7-(diethylamino)-2-benzopyrone
Inchi:	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
InchiKey:	QXAMGWKESXGGNV-UHFFFAOYSA-N
Formula:	C13H15NO2
SMILES:	CCN(CC)c1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]:	217.26
CAS:	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20571420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume