

2H-1-Benzopyran-2-one, 7-(ethylamino)-4,6-dimethyl-

Other names:	4,6-Dimethyl-7-(ethylamino)coumarin Coumarin 2 Coumarin, 7-(ethylamino)-4,6-dimethyl- 7-Ethylamino-4,6-dimethyl coumarin 7-(ethylamino)-4,6-dimethyl-2-benzopyrone
Inchi:	InChI=1S/C13H15NO2/c1-4-14-11-7-12-10(5-9(11)3)8(2)6-13(15)16-12/h5-7,14H,4H2,1-
InchiKey:	QZXAEJGHNXJTSE-UHFFFAOYSA-N
Formula:	C13H15NO2
SMILES:	CCNc1cc2oc(=O)cc(C)c2cc1C
Mol. weight [g/mol]:	217.26
CAS:	26078-25-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.81		Crippen Method
logp	2.842		Crippen Method
mcvol	172.530	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26078251&Units=SI

Legend

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

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