

Coumarin, 4,6-dimethyl-7-(methylamino)-

Other names:	4,6-dimethyl-7-(methylamino)-2-benzopyrone
Inchi:	InChI=1S/C12H13NO2/c1-7-5-12(14)15-11-6-10(13-3)8(2)4-9(7)11/h4-6,13H,1-3H3
InchiKey:	RIZOSFDXIXBLIP-UHFFFAOYSA-N
Formula:	C12H13NO2
SMILES:	CNc1cc2oc(=O)cc(C)c2cc1C
Mol. weight [g/mol]:	203.24
CAS:	26078-24-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.39		Crippen Method
logp	2.452		Crippen Method
mcvol	158.440	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26078240&Units=SI
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

Legend

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

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