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/ci990307l
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