2H-1-Benzopyran-2-one, 7-(dimethylamino)-4-methyl-

Other names:	Coumarin, 7-(dimethylamino)-4-methyl-
	Damc
	4-Methyl-7-(dimethylamino)coumarin
	7-(Dimethylamino)-4-methylcoumarin
	Coumarin 311
	FBA 52
	7-(dimethylamino)-4-methyl-2-benzopyrone
Inchi:	InChI=1S/C12H13NO2/c1-8-6-12(14)15-11-7-9(13(2)3)4-5-10(8)11/h4-7H,1-3H3
InchiKey:	GZEYLLPOQRZUDF-UHFFFAOYSA-N
Formula:	C12H13NO2
SMILES:	Cc1cc(=O)oc2cc(N(C)C)ccc12
Mol. weight [g/mol]:	203.24
CAS:	87-01-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.167		Crippen Method
mcvol	158.440	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.91	kJ/mol	416.10	NIST Webbook
sfust	56.91	J/mol×K	416.10	NIST Webbook

Sources

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

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature