4-Methyl-7-ethoxycoumarin

Other names:	2H-1-Benzopyran-2-one, 7-ethoxy-4-methyl-
	7-Ethoxy-4-methylcoumarin
	7-ethoxy-4-methyl-2H-1-benzopyran-2-one
	7-ethoxy-4-methyl-2H-benzopyran-2-one
	7-ethoxy-4-methyl-2H-chromen-2-one
	Coumarin, 7-ethoxy-4-methyl-
Inchi:	InChI=1S/C12H12O3/c1-3-14-9-4-5-10-8(2)6-12(13)15-11(10)7-9/h4-7H,3H2,1-2H3
InchiKey:	NKRISXMDKXBVRJ-UHFFFAOYSA-N
Formula:	C12H12O3
SMILES:	CCOc1ccc2c(C)cc(=O)oc2c1
Mol. weight [g/mol]:	204.22
CAS:	87-05-8

Physical Properties

Property code	Value	Unit	Source
hfus	25.81	kJ/mol	Standard molar enthalpies of formation in the crystalline phase of 7-hydroxy-4-methylcoumarin, 7-ethoxy-4-methylcoumarin, and 6-methoxy-4-methylcoumarin
log10ws	-7.45		Crippen Method
logp	2.500		Crippen Method
mcvol	154.330	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard molar enthalpies of formation in the crystalline phase of 7-hydroxy-4-methylcoumarin, 7-ethoxy-4-methylcoumarin, and 6-methoxy-4-methylcoumarin:	https://www.doi.org/10.1016/j.jct.2011.04.013
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87058&Units=SI

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume