7-Ethoxycoumarin

Other names:	2H-1-Benzopyran-2-one, 7-ethoxy- 2H-1-benzopyran-2-one, 6-methoxy-4-methyl- 6-methoxy-4-methylcoumarin Coumarin, 7-ethoxy- Ethylumbelliferone
Inchi:	InChI=1S/C11H10O3/c1-2-13-9-5-3-8-4-6-11(12)14-10(8)7-9/h3-7H,2H2,1H3
InchiKey:	LIFAQMGORKPVDH-UHFFFAOYSA-N
Formula:	C11H10O3
SMILES:	CCOc1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]:	190.20
CAS:	31005-02-4

Physical Properties

Property code	Value	Unit	Source
hfus	33.31	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	-6.97		Crippen Method
logp	2.192		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
rinpol	1771.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1754.00		NIST Webbook

Sources

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=C31005024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices