2H-1-Benzopyran-2-one, 3-methyl-

Other names:	Coumarin, 3-methyl-
	3-Methylcoumarin
	3-Methylcumarin
	3-Methyl-2H-1-benzopyran-2-one
Inchi:	InChI=1S/C10H8O2/c1-7-6-8-4-2-3-5-9(8)12-10(7)11/h2-6H,1H3
InchiKey:	VIIIJFZJKFXOGG-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	Cc1cc2ccccc2oc1=O
Mol. weight [g/mol]:	160.17
CAS:	2445-82-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	2.101		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
tb	565.70	K	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445821&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature