

2H-1-Benzopyran-2-one, 6-methyl-

Other names:	Coumarin, 6-methyl- Toncarine 6-Methylbenzopyrone 6-Methylcoumarin 6-Methylcoumarinic anhydride 6-MC 6-Methylcumarin NCI-C55812 6-Methyl-1,2-benzopyrone 6-Methyl-2H-1-benzopyran-2-one NSC 5870
Inchi:	InChI=1S/C10H8O2/c1-7-2-4-9-8(6-7)3-5-10(11)12-9/h2-6H,1H3
InchiKey:	FXFYOPQLGGEACP-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	<chem>Cc1ccc2oc(=O)ccc2c1</chem>
Mol. weight [g/mol]:	160.17
CAS:	92-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	2.101		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
ripol	1588.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	2630.00		NIST Webbook
ripol	2551.00		NIST Webbook
ripol	2630.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2551.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	576.20	K	96.70	NIST Webbook
tbrp	447.20	K	1.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C92488&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
tbrp:	Boiling point at reduced pressure

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