Coumafuryl

Other names:	2H-1-Benzopyran-2-one, 3-[1-(2-furanyl)-3-oxobutyl]-4-hydroxy-
	Coumarin, 3-(«alpha»-furylacetonyl)-4-hydroxy-
	Foumarin
	Fumarin
	Ratafin
	Cumafuryl
	Furmarin
	3-(«alpha»-Furyl-«beta»-acetylaethyl)-4-hydroxycumarin
	3-(1-Furyl-3-acetylethyl)-4-hydroxycoumarin
	4-(2-Furyl)-4-(4-hydroxy-3-coumarinyl)-2-butanone
	4-(2-Furyl)-4-(4-hydroxy-3-kumarinyl)-2-butanon
	Kill-ko rat
	Krumkil
	Kumatox
	Lurat
	Mouse blues
	Tomarin
	Coumarin, 3-(«alpha»-acetonylfurfuryl)-4-hydroxy-
	3-[1-(2-Furanyl)-3-oxobutyl]-4-hydroxy-2H-1-benzopyran-2-one
Inchi:	InChI=1S/C17H14O5/c1-10(18)9-12(13-7-4-8-21-13)15-16(19)11-5-2-3-6-14(11)22-17(15
InchiKey:	JFIXKFSJCQNGEK-UHFFFAOYSA-N
Formula:	C17H14O5
SMILES:	CC(=O)CC(c1ccco1)c1c(O)c2ccccc2oc1=O
Mol. weight [g/mol]:	298.29
CAS:	117-52-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.31		Crippen Method
logp	3.203		Crippen Method
mcvol	212.760	ml/mol	McGowan Method
tf	395.26 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.88	kJ/mol	391.80	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=C117522&Units=SI

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
tf:	Normal melting (fusion) point