Hymecromone

Other names:
2H-1-Benzopyran, 7-hydroxy-4-methyl-2-oxo-
2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-
2H-1-Benzopyren-2-one, 7-hydroxy-4-methyl-
4-MU
4-Methylumbelliferon
4-methyl-7-hydroxycoumarin
4-methylumbelliferone
7-Hydroxy-4-methyl-2-oxo-2H-1-benzopyran
7-Hydroxy-4-methyl-2-oxo-3-chromene
7-Hydroxy-4-methylcoumarin
7-hydroxy-4-methyl-2H-1-benzopyran-2-one
7-hydroxy-4-methyl-2H-chromen-2-one
Bilicante
Biliton H
Cantabilin
Cholestil
Cholonerton
Cholspasmin
Coumarin 4
Coumarin, 7-hydroxy-4-methyl-
Crodimon
Cumarote-C
Eurogale
Himecol
Hymecromon
Imecromone
LM 94
Medilla
Mendiaxon
Methylumbelliferone, «beta»
NSC 19026
NSC 9408
Omega 127
Pilot 447
Umbelliferone, 4-methyl-
bilcolic
cantabiline
«beta»-Methylumbelliferone

Inchi: InChI=1S/C10H8O3/c1-6-4-10(12)13-9-5-7(11)2-3-8(6)9/h2-5,11H,1H3

InchiKey: HSHNITRMYYLLCV-UHFFFAOYSA-N

Formula:	C10H8O3
SMILES:	Cc1cc(=O)oc2cc(O)ccc12
Mol. weight [g/mol]:	176.17
CAS:	90-33-5

Physical Properties

Property code	Value	Unit	Source
hfus	31.41	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
ie	8.47	eV	NIST Webbook
log10ws	-6.46		Crippen Method
logp	1.807		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
rinpol	2003.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.14	kJ/mol	460.70	NIST Webbook
hfust	29.14	kJ/mol	460.70	NIST Webbook
sfust	63.42	J/mol×K	460.70	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
Volumetric, Viscometric, and Refractive Index Behavior of Some Coumarin Derivatives in Aqueous Ethanol or 1-Propanol Solutions in the Temperature Range of (293.15 to 313.15) K:	https://www.doi.org/10.1021/je4003515
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature