

7H-Furo[3,2-g][1]benzopyran-7-one

Other names:	2-Propenoic acid, 3-(6-hydroxy-5-benzofuranyl)-, «delta»-lactone
	5-Benzofuranacrylic acid, 6-hydroxy-, «delta»-lactone
	6,7-Furanocoumarin
	Furo(2',3',7,6)coumarin
	Furo(4',5',6,7)coumarin
	Furo[2',3':7,6]coumarin
	Furo[2'.3':7.6]coumarin
	Furo[4',5':6,7]coumarin
	Furocoumarin
	NSC 404562
	Psoralen
	Psoralene
	Psorline-P
Inchi:	InChI=1S/C11H6O3/c12-11-2-1-7-5-8-3-4-13-9(8)6-10(7)14-11/h1-6H
InchiKey:	ZCCUUQDIBDJBTK-UHFFFAOYSA-N
Formula:	C11H6O3
SMILES:	O=c1ccc2cc3ccoc3cc2o1
Mol. weight [g/mol]:	186.17

Physical Properties

Property code	Value	Unit	Source
hf	-236.54	kJ/mol	Cheméo Relay (1.0)
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-3.74		Aqueous Solubility Prediction Method
logp	2.539		Crippen Method
mcvol	125.080	ml/mol	McGowan Method
rinpol	1805.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1847.30		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1805.00		NIST Webbook
tb	642.10	K	Cheméo Relay (1.0)
tf	436.65	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C66977&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpolar: Non-polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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