Coumarin

Other names:	1,2-Benzopyrone
	2(2H)-chromenone
	2-Oxo-1,2-benzopyran
	2-Propenoic acid, 3-(2-hydroxyphenyl)-, «delta»-lactone
	2-Propenoic acid, 3-(2-hydroxyphenyl)-, Â«deltaÂ»-lactone
	2-propenoic acid, 3-(2-hydroxyphenyl)-, .delta.-lactone
	2H-1-Benzopyran, 2-oxo-
	2H-1-Benzopyran-2-one
	2H-Benzo[b]pyran-2-one
	5,6-benzo-2-pyrone
	Benzo-«alpha»-pyrone
	Benzo-Â«alphaÂ»-pyrone
	Cinnamic acid, o-hydroxy-, «delta»-lactone
	Cinnamic acid, o-hydroxy-, Â«deltaÂ»-lactone
	Coumarinic anhydride
	Cumarin
	Kumarin
	NCI C07103
	NSC 8774
	Rattex
	Tonka bean camphor
	benzo-.alpha.-pyrone
	cis-o-Coumarinic acid lactone
	o-Hydroxycinnamic acid lactone
	o-Hydroxycinnamic lactone
	o-Hydroxyzimtsaure-lacton
Inchi:	InChI=1S/C9H6O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-6H
InchiKey:	ZYGHJZDHTFUPRJ-UHFFFAOYSA-N
Formula:	C9H6O2
SMILES:	O=c1ccc2ccccc2o1
Mol. weight [g/mol]:	146.14
CAS:	91-64-5

Physical Properties

Property code	Value	Unit	Source
chs	-4139.20 ± 1.70	kJ/mol	NIST Webbook

hf	-176.80 ± 1.80	kJ/mol	NIST Webbook
hfs	-259.90 ± 1.80	kJ/mol	NIST Webbook
hsub	83.10	kJ/mol	NIST Webbook
hsub	83.09 ± 0.22	kJ/mol	NIST Webbook
hsub	83.10	kJ/mol	NIST Webbook
hsub	95.40 ± 2.60	kJ/mol	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-1.80		Aqueous Solubility Prediction Method
logp	1.793		Crippen Method
mcvol	106.190	ml/mol	McGowan Method
rinpol	1392.00		NIST Webbook
rinpol	246.20		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1404.90		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1458.50		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1466.00		NIST Webbook
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rinpol	1397.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1418.00		NIST Webbook

rinpol	1439.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1431.00		NIST Webbook
ripol	2450.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2460.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2463.00		NIST Webbook
ripol	2458.00		NIST Webbook
ripol	2450.00		NIST Webbook
ripol	2437.00		NIST Webbook
ripol	2456.00		NIST Webbook
ripol	2451.00		NIST Webbook
ripol	2451.00		NIST Webbook
ripol	2428.00		NIST Webbook
ripol	2467.00		NIST Webbook
tb	571.20	K	NIST Webbook
tb	564.00	K	NIST Webbook
tf	343.65	K	Aqueous Solubility Prediction Method
tf	344.44	K	Determination and correlation of solubility and solution thermodynamics of coumarin in different pure solvents
tf	343.00	K	NIST Webbook
tf	343.05 ± 1.50	K	NIST Webbook
tf	340.00 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.14	kJ/mol	342.14	NIST Webbook
hfust	19.14	kJ/mol	342.14	NIST Webbook
hfust	18.63	kJ/mol	342.30	NIST Webbook
hfust	19.14	kJ/mol	342.10	NIST Webbook
hsubt	86.20	kJ/mol	323.00	NIST Webbook
hsubt	83.09	kJ/mol	298.15	NIST Webbook

hvapt	63.20	kJ/mol	421.00	NIST Webbook

Sources

Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds:	https://www.doi.org/10.1016/j.fluid.2014.10.033
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Equilibrium partitioning of drug molecules between aqueous and amino acid ester based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
Vapor-Liquid Equilibrium Behaviors of Coumarin and Vanillin in Ethanol, 1-Propanol, and 2-Propanol:	https://www.doi.org/10.1021/je0505164
Solubility of pharmaceutical compounds in ionic liquidsAna:	https://www.doi.org/10.1016/j.fluid.2013.07.020
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid:	https://www.doi.org/10.1016/j.fluid.2015.03.053
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91645&Units=SI
Determination and correlation of solubility and solution thermodynamics of coumarin in different pure solvents:	https://www.doi.org/10.1016/j.fluid.2015.03.022

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point