Rotenone

Other names:

(-)-Rotenone

(-)-cis-Rotenone

(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aH)-one,
1,2,12,12a-tetrahydro-2-«alpha»-isopropenyl-8,9-dimethoxy-

(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aH)-one,
1,2,12,12a-tetrahydro-2-Â«alphaÂ»-isopropenyl-8,9-dimethoxy-

(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aH)-one,1,2,12,12a-tetrahydro-8,9-di

(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6a«alpha»H)-one,
1,2,12,12a«alpha»-tetrahydro-2«alpha»-isopropenyl-8,9-dimethoxy-

(1)Benzopyrano(3,4-b)furo(2,3-h)(1)benzopyran-6(6aÂ«alphaÂ»H)-one,
1,2,12,12aÂ«alphaÂ»-tetrahydro-2Â«alphaÂ»-isopropenyl-8,9-dimethoxy-

(2R,2«alpha»,6a«alpha»,12a«alpha»)-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methyle

(2R,2Â«alphaÂ»,6aÂ«alphaÂ»,12aÂ«alphaÂ»)-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1

(2R,6aS,12aS)-1,2,6,6a,12,12a-hexahydro-2-isopropenyl-8,9-dimethoxychromeno[3,4-b]f

1,2,12,12a-tetrahydro-2-isopropenyl-8,9-dimethoxy[1]benzopyrano[3,4-b]furo[2,3-h][1]ben

1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-b]furo[2,3-h

2,6a,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-b]furo[2,3-

2-Isopropenyl-8,9-dimethoxy-1,2,12,12a-tetrahydrochromeno[3,4-b]furo[2,3-H]chromen-6

(6R,6a«alpha»,12a«alpha»)-
2-Isopropenyl-8,9-dimethoxy-1,2,12,12a-tetrahydrochromeno[3,4-b]furo[2,3-H]chromen-6
5'«beta»-Rotenone

(6R,6aÂ«alphaÂ»,12aÂ«alphaÂ»)-
5'Â«betaÂ»-Rotenone

Barbasco

Cenol garden dust

Chem fish

Chem-Mite

Cube extract

Cube root

Cube-Pulver

Cubor

Curex flea duster

Dactinol

Deril

Derrin

Derris

Derris (insecticide)

Derris root

Dri-kil

ENT 133

Extrax

Fish-Tox

Foliafume E.C.

Green Cross Warble Powder

Green cross warble

Haiari

Liquid Derris
Mexide
NCI-C55210
Nicouline
Noxfire
Noxfish
Nusyn-noxfish
Paraderil
Pb-nox
Powder and root
Prenfish
Prentox
Pro-nox fish
Ro-Ko
Ronone
Rotacide E.C.
Rotefive
Rotefour
Rotenon
Rotenona
Rotenox
Rotessenol
Rotocide
Synpren
Tubatoxin
Tubotoxin

Inchi:	[1]Benzopyrano[3,4-b]furo[2,3-h][1]benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-, [2R-(2A«alphaA»,6aA«alphaA»,12aA«alphaA»)]-
InchiKey:	JUVIOZPCNVVQFO-UHFFFAOYSA-N
Formula:	C23H22O6
SMILES:	C=C(C)C1Cc2c(ccc3c2OC2COc4cc(OC)c(OC)cc4C2C3=O)O1
Mol. weight [g/mol]:	394.42
CAS:	83-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-19.59	kJ/mol	Joback Method
hf	-577.91	kJ/mol	Joback Method

hfus	28.46	kJ/mol	Experimental Phase Equilibrium Data for Rotenone in Supercritical Carbon Dioxide
hvap	97.06	kJ/mol	Joback Method
log10ws	-4.42		Aqueous Solubility Prediction Method
log10ws	-4.42		Estimated Solubility Method
logp	3.703		Crippen Method
mcvol	281.450	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	3242.00		NIST Webbook
tb	1019.17	K	Joback Method
tc	1270.91	K	Joback Method
tf	438.20 ± 0.20	K	NIST Webbook
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.76	J/mol×K	1228.95	Joback Method
cpg	962.69	J/mol×K	1019.17	Joback Method
cpg	976.99	J/mol×K	1061.13	Joback Method
cpg	990.14	J/mol×K	1103.08	Joback Method
cpg	1002.25	J/mol×K	1145.04	Joback Method
cpg	1013.42	J/mol×K	1187.00	Joback Method
cpg	1033.36	J/mol×K	1270.91	Joback Method
hfust	35.64	kJ/mol	437.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.20	K	0.07	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental Phase Equilibrium Data for Rotenone in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.8b01165

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume