2H-1-Benzopyran-2-one, 4-hydroxy-3-(1,2,3,4-tetrahydro-1-naphthalenyl)-

Other names: 3-(1,2,3,4-Tetrahydro-1-naphthyl)-4-hydroxycoumarin
3-(1,2,3,4-Tetrahydro-1-naphthyl)-4-hydroxycoumarine
3-(1,2,3,4-Tetrahydro-1-naphtyl)-4-hydroxycoumarine
3-(1-Tetralyl)-4-hydroxycoumarin
3-(d-Tetralyl)-4-hydroxycoumarin
3-(«alpha»-Tetralinyl)-4-hydroxycoumarin
3-(«alpha»-Tetralyl)-4-hydroxycoumarin
3-(Â«alphaÂ»-Tetralinyl)-4-hydroxycoumarin
3-(Â«alphaÂ»-Tetralyl)-4-hydroxycoumarin
4-Hydroxy-3-(1,2,3,4-tetrahydro-1-naftyl)-cumarine
4-Hydroxy-3-(1,2,3,4-tetrahydro-1-naphthalenyl)-2H-1-benzopyran-2-one
4-Hydroxy-3-(1,2,3,4-tetrahydro-1-naphthyl)-cumarin
4-Hydroxy-3-(1,2,3,4-tetrahydro-1-naphthyl)coumarin
4-Idrossi-3-(1,2,3,4-tetraidro-1-naftil)-cumarina
BAY 25634
BAY ENE 11183 B
BAYER 25 634
Coumarin, 4-hydroxy-3-(1,2,3,4-tetrahydro-1-naphthyl)-
Coumatetralyl
Coumetralyl
Cumatetralyl
ENE 11183 B
Endox
Endrocid
Endrocide
Racumin
Raucumin 57
Rodentin

Inchi: InChI=1S/C19H16O3/c20-18-15-9-3-4-11-16(15)22-19(21)17(18)14-10-5-7-12-6-1-2-8-13

InchiKey: ULSLJYXHZDTLQK-UHFFFAOYSA-N

Formula: C19H16O3

SMILES: O=c1oc2ccccc2c(O)c1C1CCCc2ccccc21

Mol. weight [g/mol]: 292.33

CAS: 5836-29-3

Physical Properties

Property code	Value	Unit	Source

log10ws	-2.84		Aqueous Solubility Prediction Method
log10ws	-2.84		Estimated Solubility Method
logp	3.967		Crippen Method
mcvol	218.340	ml/mol	McGowan Method

Sources

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
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=C5836293&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume