

2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-

Other names:	beta-Isopropyltropolone 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-isopropyl- «beta»-Isopropyltropolon «beta»-Thujaplicin «beta»-Thujaplicine Hinokitiol 4-Isopropyltropolone 2-Hydroxy-4-isopropyl-2,4,6-cycloheptatrien-1-one Hinokitol Tropolone, 4-isopropyl- Thujaplicin, «beta» NSC 18804 2-hydroxy-4-isopropyl-2,4,6-cyclohepta-2,4,6-trien-1-one
Inchi:	InChI=1S/C10H12O2/c1-7(2)8-4-3-5-9(11)10(12)6-8/h3-7H,1-2H3,(H,11,12)
InchiKey:	FUWUEFKEXZQKKA-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)c1cccc(O)c(=O)c1
Mol. weight [g/mol]:	164.20
CAS:	499-44-5

Physical Properties

Property code	Value	Unit	Source
chs	-5309.50	kJ/mol	NIST Webbook
hfs	-340.60 ± 3.80	kJ/mol	NIST Webbook
log10ws	-1.63		Crippen Method
logp	1.876		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C499445&Units=SI>

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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