

Naphtho[2,3-b]furan-9(4H)-one, 4a,5,6,7,8,8a-hexahydro-3,4a,5-trimethyl-, [4aR-(4a«alpha»,5«alpha»,8a«alpha»)]-

Other names: Eremophilone, 7,11-dioxo-9-one-8,12-dioxo-
Euryopsonol, dehydrodeoxy-

Furannoeremophilone

Furanoeremophilone

Inchi: InChI=1S/C15H20O2/c1-9-8-17-14-11(9)7-15(3)10(2)5-4-6-12(15)13(14)16/h8,10,12H,4-

InchiKey: KLLSQGNSOCVVAN-UHFFFAOYSA-N

Formula: C15H20O2

SMILES: Cc1coc2c1CC1(C)C(C)CCCC1C2=O

Mol. weight [g/mol]: 232.32

CAS: 15404-32-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.72		Crippen Method
logp	3.769		Crippen Method
mcvol	188.470	ml/mol	McGowan Method

Sources

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=C15404327&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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