

Dehydroelsholtzia ketone

Inchi:	InChI=1S/C10H12O2/c1-7(2)6-9(11)10-8(3)4-5-12-10/h4-6H,1-3H3
InchiKey:	XWFVDCOWPBJQFH-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	<chem>CC(C)=CC(=O)c1occc1C</chem>
Mol. weight [g/mol]:	164.20
CAS:	6138-88-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	2.737		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1306.10		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1884.00		NIST Webbook

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=C6138881&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
rinpol:	Non-polar retention indices

ripol: Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/94-315-8/Dehydroelsholtzia-ketone.pdf>

Generated by Cheméo on 2025-12-05 13:57:32.912667109 +0000 UTC m=+4691250.442707773.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.