1,4:5,8-Dimethanonaphthalen-9-ol, decahydro-, stereoisomer

Inchi: InChI=1S/C12H18O/c13-12-8-3-4-9(12)11-7-2-1-6(5-7)10(8)11/h6-13H,1-5H2
InchiKey: ZPOMMBHYDITYNL-UHFFFAOYSA-N
Formula: C12H18O
SMILES: [O]C1C2CCC1C1C3CCC(C3)C21
Mol. weight [g/mol]: 178.27
CAS: 36197-17-8

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
log10ws	-6.98		Crippen Method
logp	2.488		Crippen Method
mcvol	140.220	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C36197178&Units=SI

Legend

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

Latest version available from:
https://www.chemeo.com/cid/48-031-4/1-4-5-8-Dimethanonaphthalen-9-ol-decahydro-stereoisomer.pdf

Generated by Cheméo on 2024-04-19 20:17:04.009754702 +0000 UTC m=+15847072.930332017.

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