

Cyclonona-1,2,6-triene

Inchi: InChI=1S/C9H12/c1-2-4-6-8-9-7-5-3-1/h1-2,7-8H,3-6H2/b2-1-
InchiKey: QNZNFKRCAMWGDS-UPHRSURJSA-N
Formula: C9H12
SMILES: C1=CCCC=CCCC=1
Mol. weight [g/mol]: 120.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	2.828		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
rinpol	1309.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U196999&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/23-652-2/Cyclonona-1-2-6-triene.pdf>

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