Methyl, 1,2-phenylenebis-

Inchi: InChI=1S/C8H8/c1-7-5-3-4-6-8(7)2/h3-6H,1-2H2
InchiKey: XURVRZSODRHRNK-UHFFFAOYSA-N
Formula: C8H8
SMILES: C=c1ccccc1=C
Mol. weight [g/mol]: 104.15
CAS: 32714-83-3

Physical Properties

Property code	Value	Unit	Source
ea	0.92 ± 0.01	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.507		Crippen Method
mcvol	95.520	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=C32714833&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ea: Electron affinity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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