1,6-Dioxacyclodeca-3,8-diyne

Inchi: InChI=1S/C8H8O2/c1-2-6-10-8-4-3-7-9-5-1/h5-8H2
InchiKey: VZEWQJVTGHLHHT-UHFFFAOYSA-N
Formula: C8H8O2
SMILES: C1#CCOCC#CCOC1
Mol. weight [g/mol]: 136.15
CAS: 6573-64-4

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
log10ws	-0.83		Crippen Method
logp	0.040		Crippen Method
mcvol	107.260	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=C6573644&Units=SI

Legend

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