Tetracarbon

Inchi: InChI=1S/C4/c1-2-4-3-1
InchiKey: ZJRINDVWMDPKLP-UHFFFAOYSA-N
Formula: C4
SMILES: C1=C=C=C=1
Mol. weight [g/mol]: 48.04
CAS: 12184-80-4

Physical Properties

Property code	Value	Unit	Source
ea	3.70 ± 0.10	eV	NIST Webbook
ea	2.10 ± 0.10	eV	NIST Webbook
ea	3.88 ± 0.01	eV	NIST Webbook
ie	12.54 ± 0.35	eV	NIST Webbook
ie	12.60	eV	NIST Webbook
log10ws	-0.89		Crippen Method
logp	0.620		Crippen Method
mcvol	39.160	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=C12184804&Units=SI

Legend

ea: Electron affinity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume