2-Propynylidyne

Other names: 2-Propynylidene
Inchi: InChI=1S/C3H2/c1-3-2/h1-2H
InchiKey: OUSWHEMIRJJMAW-UHFFFAOYSA-N
Formula: C3H
SMILES: [CH]C#C
Mol. weight [g/mol]: 37.04
CAS: 53590-28-6

Physical Properties

Property code	Value	Unit	Source
ea	2.00 ± 0.00	eV	NIST Webbook
ea	1.84 ± 0.00	eV	NIST Webbook
ea	1.86 ± 0.03	eV	NIST Webbook
log10ws	-0.43		Crippen Method
logp	0.331		Crippen Method
mcvol	40.230	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=C53590286&Units=SI

Legend

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