

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

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