

Propadienylidene

Inchi: InChI=1S/C3H2/c1-3-2/h1H2
InchiKey: LPUFMQSFYARLPQ-UHFFFAOYSA-N
Formula: C3H2
SMILES: [C]=C=C
Mol. weight [g/mol]: 38.05
CAS: 60731-10-4

Physical Properties

Property code	Value	Unit	Source
ea	1.80 ± 0.00	eV	NIST Webbook
ea	1.79 ± 0.01	eV	NIST Webbook
ea	1.79 ± 0.03	eV	NIST Webbook
ie	10.43 ± 0.02	eV	NIST Webbook
log10ws	-0.38		Crippen Method
logp	0.637		Crippen Method
mcvol	40.230	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C60731104&Units=SI>
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>

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

Latest version available from:

<https://www.chemeo.com/cid/53-674-5/Propadienyldene.pdf>

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