

Dicarbon

Inchi: InChI=1S/C2/c1-2
InchiKey: LBVWYGNNGGJURHQ-UHFFFAOYSA-N
Formula: C2
SMILES: [C]#[C]
Mol. weight [g/mol]: 24.02
CAS: 12070-15-4

Physical Properties

Property code	Value	Unit	Source
ea	3.27 ± 0.01	eV	NIST Webbook
ea	3.27 ± 0.02	eV	NIST Webbook
ea	3.39 ± 0.02	eV	NIST Webbook
ea	3.30 ± 0.10	eV	NIST Webbook
ea	3.54 ± 0.05	eV	NIST Webbook
ea	3.30 ± 0.20	eV	NIST Webbook
ea	2.90	eV	NIST Webbook
ea	2.90 ± 0.50	eV	NIST Webbook
ea	4.00 ± 1.00	eV	NIST Webbook
ie	11.41 ± 0.30	eV	NIST Webbook
ie	11.40 ± 0.30	eV	NIST Webbook
ie	11.92 ± 0.09	eV	NIST Webbook
ie	12.15	eV	NIST Webbook
ie	11.10 ± 0.50	eV	NIST Webbook
ie	10.90 ± 0.40	eV	NIST Webbook
ie	11.10 ± 1.00	eV	NIST Webbook
ie	12.00 ± 0.60	eV	NIST Webbook
ie	13.00	eV	NIST Webbook
log10ws	0.33		Crippen Method
logp	0.163		Crippen Method
mccvol	26.140	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C12070154&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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<https://www.chemeo.com/cid/16-682-7/Dicarbon.pdf>

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