Carbon trimer

Other names: Carbon trimer
Inchi: InChI=1S/C3/c1-3-2
InchiKey: NVLRFXKSQQPKAD-UHFFFAOYSA-N
Formula: C3
SMILES: [C]=C=[C]
Mol. weight [g/mol]: 36.03

Physical Properties

Property code	Value	Unit	Source
affp	767.00	kJ/mol	NIST Webbook
basg	736.30	kJ/mol	NIST Webbook
ea	2.50 ± 1.00	eV	NIST Webbook
ea	1.95 ± 0.10	eV	NIST Webbook
ea	1.98 ± 0.02	eV	NIST Webbook
ea	2.00 ± 0.03	eV	NIST Webbook
ie	12.10 ± 0.30	eV	NIST Webbook
ie	12.60 ± 0.60	eV	NIST Webbook
ie	13.00 ± 0.10	eV	NIST Webbook
ie	12.10 ± 0.20	eV	NIST Webbook
ie	11.10 ± 0.50	eV	NIST Webbook
logp	0.318		Crippen Method
mcvol	35.930	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C12075353&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume