Benzyne

Inchi: InChI=1S/C6H4/c1-2-4-6-5-3-1/h1-4H
InchiKey: KLYCPFXDDDMZNQ-UHFFFAOYSA-N
Formula: C6H4
SMILES: c1ccccc#1
Mol. weight [g/mol]: 76.10
CAS: 462-80-6

Physical Properties

Property code	Value	Unit	Source
affp	841.00	kJ/mol	NIST Webbook
basg	808.50	kJ/mol	NIST Webbook
ea	1.26 ± 0.01	eV	NIST Webbook
ea	0.56 ± 0.01	eV	NIST Webbook
ea	1.25 ± 0.02	eV	NIST Webbook
ea	0.56 ± 0.01	eV	NIST Webbook
ea	0.56 ± 0.01	eV	NIST Webbook
hf	440.00 ± 10.00	kJ/mol	NIST Webbook
hf	440.00 ± 10.00	kJ/mol	NIST Webbook
hf	490.00 ± 20.00	kJ/mol	NIST Webbook
ie	9.03 ± 0.05	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
ie	9.80 ± 0.20	eV	NIST Webbook
ie	9.50 ± 0.20	eV	NIST Webbook
log10ws	-0.84		Crippen Method
logp	1.287		Crippen Method
mcvol	67.340	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=C462806&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
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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