

Fulminic acid

Inchi: InChI=1S/CHNO/c1-2-3/h1H
InchiKey: UXKUODQYLDZXDL-UHFFFAOYSA-N
Formula: CHNO
SMILES: C#[N+][O-]
Mol. weight [g/mol]: 43.02
CAS: 506-85-4

Physical Properties

Property code	Value	Unit	Source
affp	758.00	kJ/mol	NIST Webbook
basg	725.50	kJ/mol	NIST Webbook
ie	10.83	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	0.447		Crippen Method
mcvol	32.200	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=C506854&Units=SI>

Legend

affp: Proton affinity
basg: Gas basicity
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/73-648-2/Fulminic-acid.pdf>

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