

Ethyl diazoacetate

Other names:	Acetic acid, diazo-, ethyl ester Diazoacetic acid ethyl ester Diazoacetic ester Ethoxycarbonyldiazomethane Daae Diazoessigsaeure-aethylester EDA Ethyl 2-diazoacetate
Inchi:	InChI=1S/C4H6N2O2/c1-2-8-4(7)3-6-5/h3H,2H2,1H3
InchiKey:	YVPJCJLMRRTDMQ-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	CCOC(=O)C=[N+]=[N-]
Mol. weight [g/mol]:	114.10
CAS:	623-73-4

Physical Properties

Property code	Value	Unit	Source
ea	0.85 ± 0.09	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	-0.150		Crippen Method
mcvol	86.020	ml/mol	McGowan Method
rinpole	867.00		NIST Webbook
rinpole	834.00		NIST Webbook
rinpole	840.00		NIST Webbook
rinpole	840.00		NIST Webbook

Sources

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=C623734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ea:	Electron affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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