

1-Diazopentan-2-one

Inchi:	InChI=1S/C5H8N2O/c1-2-3-5(8)4-7-6/h4H,2-3H2,1H3
InchiKey:	DLRGYMDHPDGMHJ-UHFFFAOYSA-N
Formula:	C5H8N2O
SMILES:	CCCC(=O)C=[N+]=[N-]
Mol. weight [g/mol]:	112.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	0.656		Crippen Method
mcvol	94.240	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R632930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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/98-406-3/1-Diazopentan-2-one.pdf>

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