

2-Propanone,1-chloro-3-dizao

Inchi: InChI=1S/C3H3ClN2O/c4-1-3(7)2-6-5/h2H,1H2
InchiKey: QQRZDPCAMOLWBA-UHFFFAOYSA-N
Formula: C3H3ClN2O
SMILES: [N-]=[N+]=CC(=O)CCl
Mol. weight [g/mol]: 118.52
CAS: 20485-53-4

Physical Properties

Property code	Value	Unit	Source
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	0.095		Crippen Method
mcvol	78.300	ml/mol	McGowan Method

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=C20485534&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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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