

2-Propanone,1,1,1-trichloro-3-dizao

Inchi: InChI=1S/C3HCl3N2O/c4-3(5,6)2(9)1-8-7/h1H
InchiKey: ZDZWSRDKBMPXHR-UHFFFAOYSA-N
Formula: C3HCl3N2O
SMILES: [N-]=[N+]=CC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 187.41
CAS: 20485-55-6

Physical Properties

Property code	Value	Unit	Source
ie	9.95 ± 0.06	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	1.226		Crippen Method
mcvol	102.780	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20485556&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

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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