3-Methyl-2,5-oxazolidine-dione

Other names: N-Methyloxazole, 2,5-dione
Inchi: InChI=1S/C4H5NO3/c1-5-2-3(6)8-4(5)7/h2H2,1H3
InchiKey: PMPAXURTFMSZSN-UHFFFAOYSA-N
Formula: C4H5NO3
SMILES: CN1CC(=O)OC1=O
Mol. weight [g/mol]: 115.09
CAS: 5840-76-6

Physical Properties

Property code	Value	Unit	Source
chs	-1688.20 ± 2.90	kJ/mol	NIST Webbook
hfs	-600.40 ± 2.90	kJ/mol	NIST Webbook
log10ws	0.42		Crippen Method
logp	-0.405		Crippen Method
mcvol	75.350	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5840766&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume