

1,3-Dioxol-2-one

Other names:	Vinylene carbonate Carbonic acid, cyclic vinylene ester
Inchi:	InChI=1S/C3H2O3/c4-3-5-1-2-6-3/h1-2H
InchiKey:	VAYTZRYEBVHVLE-UHFFFAOYSA-N
Formula:	C3H2O3
SMILES:	O=c1occo1
Mol. weight [g/mol]:	86.05
CAS:	872-36-6

Physical Properties

Property code	Value	Unit	Source
chl	-1006.50 ± 2.10	kJ/mol	NIST Webbook
hf	-418.61	kJ/mol	NIST Webbook
hfl	-460.00 ± 2.00	kJ/mol	NIST Webbook
hvac	41.30 ± 2.10	kJ/mol	NIST Webbook
hvac	41.40	kJ/mol	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	11.91	eV	NIST Webbook
log10ws	-8.36		Crippen Method
logp	0.233		Crippen Method
mccol	51.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	46.90	kJ/mol	329.00	NIST Webbook
hvapt	41.30	kJ/mol	354.00	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=C872366&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

chl: Standard liquid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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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