

4-Chloro-1,3-dioxolan-2-one

Other names:	1,3-Dioxolan-2-one, 4-chloro- Carbonic acid, cyclic chloroethylene ester 1,2-Ethanediol, 1-chloro-, cyclic carbonate Chloroethylene carbonate Cyclic chloroethylene carbonate 4-Chloro-1,3-dioxolane-2-one Carbonic acid, cyclic 1-chloroethylene ester
Inchi:	InChI=1S/C3H3ClO3/c4-2-1-6-3(5)7-2/h2H,1H2
InchiKey:	OYOKPDLAMOMTEE-UHFFFAOYSA-N
Formula:	C3H3ClO3
SMILES:	O=C1OCC(Cl)O1
Mol. weight [g/mol]:	122.51
CAS:	3967-54-2

Physical Properties

Property code	Value	Unit	Source
gf	-295.83	kJ/mol	Joback Method
hf	-462.21	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	40.18	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.718		Crippen Method
mcvol	67.820	ml/mol	McGowan Method
pc	5519.63	kPa	Joback Method
tb	442.47	K	Joback Method
tc	675.15	K	Joback Method
tf	285.75	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.60	J/mol×K	442.47	Joback Method
cpg	135.43	J/mol×K	481.25	Joback Method

cpg	142.97	J/mol×K	520.03	Joback Method
cpg	150.19	J/mol×K	558.81	Joback Method
cpg	157.08	J/mol×K	597.59	Joback Method
cpg	163.61	J/mol×K	636.37	Joback Method
cpg	169.77	J/mol×K	675.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3967542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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