

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

Physical Properties

Property code	Value	Unit	Source
hf	-582.56	kJ/mol	Cheméo Relay (1.0)
hfus	17.13	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Cheméo Relay (1.0)
logp	0.718		Crippen Method
mcvol	67.820	ml/mol	McGowan Method
tb	502.94	K	Cheméo Relay (1.0)
tf	309.64	K	Cheméo Relay (1.0)

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
cpl	238.00	J/mol×K	298.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3967542&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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