

Acetyl chloride, 2,2'-oxybis-

Other names:	Diglycolyl chloride Oxydiacetyl dichloride Diglycolic dichloride
Inchi:	InChI=1S/C4H4Cl2O3/c5-3(7)1-9-2-4(6)8/h1-2H2
InchiKey:	GTZXSBQC�BNWPK-UHFFFAOYSA-N
Formula:	C4H4Cl2O3
SMILES:	O=C(Cl)COCC(=O)Cl
Mol. weight [g/mol]:	170.98
CAS:	21062-20-4

Physical Properties

Property code	Value	Unit	Source
gf	-403.90	kJ/mol	Joback Method
hf	-514.75	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.534		Crippen Method
mcvol	100.710	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinsol	1053.40		NIST Webbook
tb	495.94	K	Joback Method
tc	701.16	K	Joback Method
tf	316.77	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.77	J/molxK	495.94	Joback Method
cpg	185.76	J/molxK	530.14	Joback Method
cpg	191.48	J/molxK	564.35	Joback Method
cpg	196.92	J/molxK	598.55	Joback Method
cpg	202.09	J/molxK	632.75	Joback Method

cpg	206.97	J/mol×K	666.96	Joback Method
cpg	211.57	J/mol×K	701.16	Joback Method
dvisc	0.0025238	Paxs	316.77	Joback Method
dvisc	0.0016139	Paxs	346.63	Joback Method
dvisc	0.0011078	Paxs	376.49	Joback Method
dvisc	0.0008037	Paxs	406.36	Joback Method
dvisc	0.0006093	Paxs	436.22	Joback Method
dvisc	0.0004786	Paxs	466.08	Joback Method
dvisc	0.0003870	Paxs	495.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21062204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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