

Pyruvyl chloride or 2-oxo-propionyl chloride

Inchi:	InChI=1S/C3H3ClO2/c1-2(5)3(4)6/h1H3
InchiKey:	AUUTXOKCFQTKPL-UHFFFAOYSA-N
Formula:	C3H3ClO2
SMILES:	CC(=O)C(=O)Cl
Mol. weight [g/mol]:	106.51
CAS:	5704-66-5

Physical Properties

Property code	Value	Unit	Source
gf	-295.39	kJ/mol	Joback Method
hf	-346.15	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	40.15	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.341		Crippen Method
mcvol	68.510	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
tb	413.21	K	Joback Method
tc	615.85	K	Joback Method
tf	253.35	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.97	J/molxK	413.21	Joback Method
cpg	111.80	J/molxK	446.98	Joback Method
cpg	116.39	J/molxK	480.76	Joback Method
cpg	120.76	J/molxK	514.53	Joback Method
cpg	124.90	J/molxK	548.30	Joback Method
cpg	128.82	J/molxK	582.08	Joback Method
cpg	132.52	J/molxK	615.85	Joback Method
dvisc	0.0030071	Paxs	253.35	Joback Method
dvisc	0.0018758	Paxs	279.99	Joback Method

dvisc	0.0012700	Paxs	306.64	Joback Method
dvisc	0.0009152	Paxs	333.28	Joback Method
dvisc	0.0006923	Paxs	359.92	Joback Method
dvisc	0.0005443	Paxs	386.57	Joback Method
dvisc	0.0004414	Paxs	413.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5704665&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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