Propanoyl chloride, 2,2-dichloro-

Other names:	Propionyl chloride, 2,2-dichloro- «alpha»,«alpha»-Dichloropropionyl chloride 2,2-Dichloropropionyl chloride 2,2-Dichloropropanoyl chloride
Inchi:	InChI=1S/C3H3Cl3O/c1-3(5,6)2(4)7/h1H3
InchiKey:	IPKCHUGFUGHNRZ-UHFFFAOYSA-N
Formula:	C3H3Cl3O
SMILES:	CC(Cl)(Cl)C(=O)Cl
Mol. weight [g/mol]:	161.41
CAS:	26073-26-7

Physical Properties

Property code	Value	Unit	Source
gf	-187.49	kJ/mol	Joback Method
hf	-273.80	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.946		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	430.97	K	Joback Method
tc	650.04	K	Joback Method
tf	265.68	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.59	J/mol×K	430.97	Joback Method
cpg	146.38	J/mol×K	467.48	Joback Method
cpg	151.65	J/mol×K	503.99	Joback Method
cpg	156.44	J/mol×K	540.51	Joback Method
cpg	160.78	J/mol×K	577.02	Joback Method

cpg	164.71	J/mol×K	613.53	Joback Method
cpg	168.25	J/mol×K	650.04	Joback Method
dvisc	0.0048742	Pa×s	265.68	Joback Method
dvisc	0.0027744	Pa×s	293.23	Joback Method
dvisc	0.0017397	Pa×s	320.78	Joback Method
dvisc	0.0011745	Pa×s	348.33	Joback Method
dvisc	0.0008399	Pa×s	375.87	Joback Method
dvisc	0.0006287	Pa×s	403.42	Joback Method
dvisc	0.0004884	Pa×s	430.97	Joback Method

Sources

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=C26073267&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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