Propanoyl chloride, 2,2-dimethyl-

Other names:	Propanoyl chloride, 2,2-dimethyl-
	Neopentanoyl chloride
	Pivalic acid chloride
	Pivalolyl chloride
	Pivaloyl chloride
	Trimethylacetyl chloride
	2,2-Dimethylpropanoyl chloride
	2,2-Dimethylpropionyl chloride
	Acetyl chloride, trimethyl-
	UN 2438
	2,2,2-Trimethylacetyl chloride
Inchi:	InChI=1S/C5H9ClO/c1-5(2,3)4(6)7/h1-3H3
InchiKey:	JVSFQJZRHXAUGT-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	CC(C)(C)C(=O)Cl
Mol. weight [g/mol]:	120.58

Physical Properties

Property code	Value	Unit	Source
af	0.2916		Cheméo Relay (1.0)
gf	-146.79	kJ/mol	Joback Method
hf	-321.91	kJ/mol	Cheméo Relay (1.0)
hfus	7.09	kJ/mol	Joback Method
hvap	32.10	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	1.798		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	377.00 ± 2.00	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tb	376.00 ± 1.00	K	NIST Webbook
tb	378.70	K	NIST Webbook
tc	543.47	K	Cheméo Relay (1.0)
tf	243.59	K	Cheméo Relay (1.0)
vc	0.347	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.29	J/mol×K	401.87	Joback Method
cpg	178.04	J/mol×K	435.07	Joback Method
cpg	187.21	J/mol×K	468.27	Joback Method
cpg	195.82	J/mol×K	501.47	Joback Method
cpg	203.89	J/mol×K	534.68	Joback Method
cpg	211.47	J/mol×K	567.88	Joback Method
cpg	218.56	J/mol×K	601.08	Joback Method
dvisc	0.0059669	Pa×s	228.38	Joback Method
dvisc	0.0029388	Pa×s	257.30	Joback Method
dvisc	0.0016700	Pa×s	286.21	Joback Method
dvisc	0.0010528	Pa×s	315.12	Joback Method
dvisc	0.0007172	Pa×s	344.04	Joback Method
dvisc	0.0005185	Pa×s	372.96	Joback Method
dvisc	0.0003928	Pa×s	401.87	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3282302&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

Legend

af: Acentric Factor
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
ie:	Ionization energy
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