2-Propanol, 1,1,1-trichloro-

Other names:	Isopral
	Trichloro-2-propanol
	1,1,1-Trichloro-2-propanol
	1,1,1-Trichloroisopropyl alcohol
	2,2,2-Trichloro-1-methylethanol
	Trichloroisopropanol
	1,1,1-trichloropropan-2-ol
Inchi:	InChI=1S/C3H5Cl3O/c1-2(7)3(4,5)6/h2,7H,1H3
InchiKey:	HCMBPASAOZIEDZ-UHFFFAOYSA-N
Formula:	C3H5Cl3O
SMILES:	CC(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	163.43
CAS:	76-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-197.83	kJ/mol	Joback Method
hf	-318.73	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	50.42	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.737		Crippen Method
mcvol	95.720	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	912.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	468.84	K	Joback Method
tc	668.42	K	Joback Method
tf	321.00 ± 5.00	K	NIST Webbook
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.06	J/mol×K	468.84	Joback Method
cpg	189.83	J/mol×K	635.16	Joback Method
cpg	185.67	J/mol×K	601.90	Joback Method
cpg	181.15	J/mol×K	568.63	Joback Method
cpg	176.22	J/mol×K	535.37	Joback Method
cpg	170.87	J/mol×K	502.10	Joback Method
cpg	193.65	J/mol×K	668.42	Joback Method
dvisc	0.0002727	Pa×s	468.84	Joback Method
dvisc	0.0004618	Pa×s	434.30	Joback Method
dvisc	0.0008565	Pa×s	399.75	Joback Method
dvisc	0.0017856	Pa×s	365.21	Joback Method
dvisc	0.0043403	Pa×s	330.66	Joback Method
dvisc	0.0129794	Pa×s	296.12	Joback Method
dvisc	0.0518380	Pa×s	261.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76006&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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