Propane, 1,2,3-trichloro-2-methyl-

Other names: 1,2,3-Trichloro-2-methylpropane
1,2,3-Trichloroisobutane
Inchi: InChI=1S/C4H7Cl3/c1-4(7,2-5)3-6/h2-3H2,1H3
InchiKey: XMCSILBVFPYTLC-UHFFFAOYSA-N
Formula: C4H7Cl3
SMILES: CC(Cl)(CCl)CCl
Mol. weight [g/mol]: 161.46
CAS: 1871-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-50.15	kJ/mol	Joback Method
hf	-181.86	kJ/mol	Joback Method
hfus	11.29	kJ/mol	Joback Method
hvap	36.36	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.462		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	918.00		NIST Webbook
tb	435.15 ± 4.00	K	NIST Webbook
tb	435.15 ± 4.00	K	NIST Webbook
tb	435.70 ± 2.00	K	NIST Webbook
tc	603.44	K	Joback Method
tf	227.02	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.83	J/mol×K	399.98	Joback Method
cpg	174.12	J/mol×K	433.89	Joback Method
cpg	181.85	J/mol×K	467.80	Joback Method
cpg	189.02	J/mol×K	501.71	Joback Method

cpg	195.69	J/mol×K	535.62	Joback Method
cpg	201.87	J/mol×K	569.53	Joback Method
cpg	207.60	J/mol×K	603.44	Joback Method
dvisc	0.0066063	Pa×s	227.02	Joback Method
dvisc	0.0032302	Pa×s	255.85	Joback Method
dvisc	0.0018257	Pa×s	284.67	Joback Method
dvisc	0.0011461	Pa×s	313.50	Joback Method
dvisc	0.0007781	Pa×s	342.33	Joback Method
dvisc	0.0005611	Pa×s	371.15	Joback Method
dvisc	0.0004241	Pa×s	399.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52332e+01
Coeff. B	-3.95374e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	327.22
Temperature range (K), max.	463.83

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1871585&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume