Propane, 1,1,1-trichloro-

Other names: 1,1,1-Trichloropropane
Inchi: InChI=1S/C3H5Cl3/c1-2-3(4,5)6/h2H2,1H3
InchiKey: AVGQTJUPLKNPQP-UHFFFAOYSA-N
Formula: C3H5Cl3
SMILES: CCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 147.43
CAS: 7789-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-58.57	kJ/mol	Joback Method
hf	-161.22	kJ/mol	Joback Method
hfus	8.70	kJ/mol	Joback Method
hvap	34.13	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.767		Crippen Method
mcvol	89.850	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	736.00		NIST Webbook
rinpol	736.00		NIST Webbook
tb	420.65	K	NIST Webbook
tb	381.20	K	NIST Webbook
tb	378.00 ± 3.00	K	NIST Webbook
tb	380.65 ± 3.00	K	NIST Webbook
tb	379.65 ± 4.00	K	NIST Webbook
tb	420.65	K	NIST Webbook
tc	582.27	K	Joback Method
tf	215.75	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.76	J/mol×K	582.27	Joback Method

cpg	161.24	J/mol×K	548.07	Joback Method
cpg	156.31	J/mol×K	513.88	Joback Method
cpg	150.97	J/mol×K	479.68	Joback Method
cpg	145.16	J/mol×K	445.49	Joback Method
cpg	138.87	J/mol×K	411.29	Joback Method
cpg	132.07	J/mol×K	377.10	Joback Method
dvisc	0.0066287	Pa×s	215.75	Joback Method
dvisc	0.0004581	Pa×s	377.10	Joback Method
dvisc	0.0006027	Pa×s	350.21	Joback Method
dvisc	0.0008300	Pa×s	323.32	Joback Method
dvisc	0.0012113	Pa×s	296.43	Joback Method
dvisc	0.0019064	Pa×s	269.53	Joback Method
dvisc	0.0033176	Pa×s	242.64	Joback Method
hvapt	38.80	kJ/mol	313.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39107e+01
Coeff. B	-3.19144e+03
Coeff. C	-4.65540e+01
Temperature range (K), min.	280.82
Temperature range (K), max.	417.68

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7789891&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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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