

Propane, 1,2,2-trichloro-

Other names:	1,2,2-Trichloropropane
Inchi:	InChI=1S/C3H5Cl3/c1-3(5,6)2-4/h2H2,1H3
InchiKey:	DAIIXVPKQATIMF-UHFFFAOYSA-N
Formula:	C3H5Cl3
SMILES:	CC(Cl)(Cl)CCl
Mol. weight [g/mol]:	147.43
CAS:	3175-23-3

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	-2.14		Crippen Method
logp	2.419		Crippen Method
mcvol	89.850	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	781.00		NIST Webbook
rinpol	781.00		NIST Webbook
tb	397.20	K	NIST Webbook
tb	396.15 ± 2.00	K	NIST Webbook
tb	397.15 ± 3.00	K	NIST Webbook
tb	395.00 ± 1.50	K	NIST Webbook
tb	400.00 ± 3.00	K	NIST Webbook
tc	582.27	K	Joback Method
tf	215.75	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.07	J/mol×K	377.10	Joback Method
cpg	161.24	J/mol×K	548.07	Joback Method

cpg	156.31	J/molxK	513.88	Joback Method
cpg	150.97	J/molxK	479.68	Joback Method
cpg	145.16	J/molxK	445.49	Joback Method
cpg	138.87	J/molxK	411.29	Joback Method
cpg	165.76	J/molxK	582.27	Joback Method
dvisc	0.0004581	Paxs	377.10	Joback Method
dvisc	0.0006027	Paxs	350.21	Joback Method
dvisc	0.0008300	Paxs	323.32	Joback Method
dvisc	0.0012113	Paxs	296.43	Joback Method
dvisc	0.0019064	Paxs	269.53	Joback Method
dvisc	0.0033176	Paxs	242.64	Joback Method
dvisc	0.0066287	Paxs	215.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48633e+01
Coeff. B	-3.54394e+03
Coeff. C	-5.12800e+01
Temperature range (K), min.	294.42
Temperature range (K), max.	422.30

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3175233&Units=SI>

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
mccvol:	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

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