Propane, 1,2,3-trichloro-2-(chloromethyl)-

Other names: 1,2,3-trichloro-2-(chloromethyl)propane
Inchi: InChI=1S/C4H6Cl4/c5-1-4(8,2-6)3-7/h1-3H2
InchiKey: CFLWPMRPCYBIIS-UHFFFAOYSA-N
Formula: C4H6Cl4
SMILES: ClCC(Cl)(CCl)CCl
Mol. weight [g/mol]: 195.90
CAS: 18963-00-3

Physical Properties

Property code	Value	Unit	Source
gf	-62.08	kJ/mol	Joback Method
hf	-197.60	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	40.74	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.680		Crippen Method
mcvol	116.180	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
tb	481.00 ± 6.00	K	NIST Webbook
tc	648.40	K	Joback Method
tf	256.94	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.66	J/mol×K	437.41	Joback Method
cpg	220.63	J/mol×K	613.23	Joback Method
cpg	215.09	J/mol×K	578.07	Joback Method
cpg	209.05	J/mol×K	542.90	Joback Method
cpg	202.50	J/mol×K	507.74	Joback Method
cpg	195.38	J/mol×K	472.57	Joback Method

cpg	225.73	J/mol×K	648.40	Joback Method
dvisc	0.0004168	Pa×s	437.41	Joback Method
dvisc	0.0005472	Pa×s	407.33	Joback Method
dvisc	0.0007503	Pa×s	377.25	Joback Method
dvisc	0.0010867	Pa×s	347.18	Joback Method
dvisc	0.0016885	Pa×s	317.10	Joback Method
dvisc	0.0028774	Pa×s	287.02	Joback Method
dvisc	0.0055551	Pa×s	256.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48307e+01
Coeff. B	-4.13861e+03
Coeff. C	-7.57440e+01
Temperature range (K), min.	360.32
Temperature range (K), max.	514.72

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18963003&Units=SI

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

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