

1,1,3-Trichloropropane

Inchi:	InChI=1S/C3H5Cl3/c4-2-1-3(5)6/h3H,1-2H2
InchiKey:	URWHLZCXYCQNSY-UHFFFAOYSA-N
Formula:	C3H5Cl3
SMILES:	CICCC(Cl)Cl
Mol. weight [g/mol]:	147.43
CAS:	20395-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-63.85	kJ/mol	Joback Method
hf	-157.75	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.419		Crippen Method
mcvol	89.850	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	420.00 ± 3.00	K	NIST Webbook
tb	416.65 ± 3.00	K	NIST Webbook
tb	421.15 ± 2.00	K	NIST Webbook
tb	418.70 ± 0.50	K	NIST Webbook
tc	576.15	K	Joback Method
tf	214.17 ± 0.60	K	NIST Webbook
vc	0.344	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.24	J/mol×K	379.89	Joback Method
cpg	136.05	J/mol×K	412.60	Joback Method
cpg	141.56	J/mol×K	445.31	Joback Method
cpg	146.78	J/mol×K	478.02	Joback Method
cpg	151.72	J/mol×K	510.73	Joback Method
cpg	156.39	J/mol×K	543.44	Joback Method

cpg	160.80	J/mol×K	576.15	Joback Method
dvisc	0.0061584	Paxs	198.33	Joback Method
dvisc	0.0028685	Paxs	228.59	Joback Method
dvisc	0.0015974	Paxs	258.85	Joback Method
dvisc	0.0010055	Paxs	289.11	Joback Method
dvisc	0.0006910	Paxs	319.37	Joback Method
dvisc	0.0005067	Paxs	349.63	Joback Method
dvisc	0.0003904	Paxs	379.89	Joback Method
hvapt	41.80	kJ/mol	396.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20395259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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