

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

Inchi:	InChI=1S/C4H7Cl3/c1-4(2,7)3(5)6/h3H,1-2H3
InchiKey:	FRRHZKFKOHHEJR-UHFFFAOYSA-N
Formula:	C4H7Cl3
SMILES:	CC(C)(Cl)C(Cl)Cl
Mol. weight [g/mol]:	161.46
CAS:	29559-52-2

Physical Properties

Property code	Value	Unit	Source
gf	-52.59	kJ/mol	Joback Method
hf	-187.14	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.807		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	399.54	K	Joback Method
tc	608.09	K	Joback Method
tf	212.02	K	Joback Method
vc	0.390	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.86	J/mol×K	399.54	Joback Method
cpg	203.10	J/mol×K	573.33	Joback Method
cpg	196.74	J/mol×K	538.57	Joback Method
cpg	189.88	J/mol×K	503.81	Joback Method
cpg	182.46	J/mol×K	469.06	Joback Method
cpg	174.47	J/mol×K	434.30	Joback Method
cpg	208.98	J/mol×K	608.09	Joback Method

dvisc	0.0004093	Paxs	399.54	Joback Method
dvisc	0.0005605	Paxs	368.29	Joback Method
dvisc	0.0008134	Paxs	337.03	Joback Method
dvisc	0.0012740	Paxs	305.78	Joback Method
dvisc	0.0022098	Paxs	274.53	Joback Method
dvisc	0.0044160	Paxs	243.27	Joback Method
dvisc	0.0108227	Paxs	212.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29559522&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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