1-Propene, 1,1,3-trichloro-2-methyl-

Other names: Propene, 1,1,3-trichloro-2-methyl-
Inchi: InChI=1S/C4H5Cl3/c1-3(2-5)4(6)7/h2H2,1H3
InchiKey: GVFGURPOQVIHNM-UHFFFAOYSA-N
Formula: C4H5Cl3
SMILES: CC(CCl)=C(Cl)Cl
Mol. weight [g/mol]: 159.44
CAS: 31702-33-7

Physical Properties

Property code	Value	Unit	Source
gf	10.13	kJ/mol	Joback Method
hf	-75.47	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	37.77	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.934		Crippen Method
mcvol	99.640	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
tb	427.00 ± 8.00	K	NIST Webbook
tc	615.84	K	Joback Method
tf	191.60	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.79	J/mol×K	407.13	Joback Method
cpg	154.55	J/mol×K	441.91	Joback Method
cpg	160.85	J/mol×K	476.70	Joback Method
cpg	166.71	J/mol×K	511.48	Joback Method
cpg	172.16	J/mol×K	546.27	Joback Method
cpg	177.24	J/mol×K	581.05	Joback Method

cpg	181.97	J/mol×K	615.84	Joback Method

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=C31702337&Units=SI

Legend

cpg:	Ideal gas heat capacity
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