(E)-1-Propene, 1,3,3-trichloro-2-methyl

Inchi: InChI=1S/C4H5Cl3/c1-3(2-5)4(6)7/h2,4H,1H3/b3-2+
InchiKey: RPKXMPUNLARZKR-NSCUHMNNSA-N
Formula: C4H5Cl3
SMILES: CC(=CCl)C(Cl)Cl
Mol. weight [g/mol]: 159.44

Physical Properties

Property code	Value	Unit	Source
gf	16.24	kJ/mol	Joback Method
hf	-70.96	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	37.30	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.933		Crippen Method
mcvol	99.640	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	894.00		NIST Webbook
tb	406.81	K	Joback Method
tc	616.31	K	Joback Method
tf	190.56	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.87	J/mol×K	406.81	Joback Method
cpg	154.80	J/mol×K	441.73	Joback Method
cpg	161.25	J/mol×K	476.64	Joback Method
cpg	167.26	J/mol×K	511.56	Joback Method
cpg	172.84	J/mol×K	546.48	Joback Method
cpg	178.03	J/mol×K	581.40	Joback Method
cpg	182.86	J/mol×K	616.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R12412&Units=SI
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

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