Propanol, 3,3,3-trichloro-2-methyl-

Inchi: InChI=1S/C4H7Cl3O/c1-3(2-8)4(5,6)7/h3,8H,2H2,1H3
InchiKey: JQQYPQBEPCDDEG-UHFFFAOYSA-N
Formula: C4H7Cl3O
SMILES: CC(CO)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 177.46
CAS: 29903-32-0

Physical Properties

Property code	Value	Unit	Source
gf	-189.41	kJ/mol	Joback Method
hf	-339.37	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.985		Crippen Method
mcvol	109.810	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	491.72	K	Joback Method
tc	688.79	K	Joback Method
tf	272.84	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.17	J/mol×K	491.72	Joback Method
cpg	210.21	J/mol×K	524.56	Joback Method
cpg	216.73	J/mol×K	557.41	Joback Method
cpg	222.79	J/mol×K	590.25	Joback Method
cpg	228.41	J/mol×K	623.10	Joback Method
cpg	233.61	J/mol×K	655.94	Joback Method
cpg	238.44	J/mol×K	688.79	Joback Method
dvisc	0.0398959	Pa×s	272.84	Joback Method
dvisc	0.0100091	Pa×s	309.32	Joback Method

dvisc	0.0033618	Pa×s	345.80	Joback Method
dvisc	0.0013905	Pa×s	382.28	Joback Method
dvisc	0.0006708	Pa×s	418.76	Joback Method
dvisc	0.0003637	Pa×s	455.24	Joback Method
dvisc	0.0002159	Pa×s	491.72	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=C29903320&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume