3-CHLORO-2,2-DIMETHYL-1-PROPANOL

Other names: 1-Propanol, 3-chloro-2,2-dimethyl-
3-chloro-2,2-dimethylpropan-1-ol
Inchi: InChI=1S/C5H11ClO/c1-5(2,3-6)4-7/h7H,3-4H2,1-2H3
InchiKey: CAZPRAORHCOIHC-UHFFFAOYSA-N
Formula: C5H11ClO
SMILES: CC(C)(CO)CCl
Mol. weight [g/mol]: 122.59

Physical Properties

Property code	Value	Unit	Source
af	0.5590		Cheméo Relay (1.0)
gf	-154.69	kJ/mol	Joback Method
hf	-356.82	kJ/mol	Cheméo Relay (1.0)
hfus	9.58	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-0.96		Cheméo Relay (1.0)
logp	1.244		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
tb	439.15	K	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of 3,3-Dimethyloxetane + Methyl Cyclohexane and 3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa
tc	649.58	K	Cheméo Relay (1.0)
tf	309.11	K	Cheméo Relay (1.0)
vc	0.349	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.35	J/mol×K	589.24	Joback Method

cpg	244.17	J/mol×K	619.06	Joback Method
cpg	205.84	J/mol×K	469.99	Joback Method
cpg	214.39	J/mol×K	499.81	Joback Method
cpg	222.48	J/mol×K	529.62	Joback Method
cpg	230.12	J/mol×K	559.43	Joback Method
cpg	196.80	J/mol×K	440.18	Joback Method
dvisc	0.0050824	Pa×s	306.24	Joback Method
dvisc	0.0163368	Pa×s	272.75	Joback Method
dvisc	0.0728117	Pa×s	239.27	Joback Method
dvisc	0.0019904	Pa×s	339.72	Joback Method
dvisc	0.0009223	Pa×s	373.21	Joback Method
dvisc	0.0004850	Pa×s	406.69	Joback Method
dvisc	0.0002813	Pa×s	440.18	Joback Method
pvap	101.30	kPa	439.15	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of 3,3-Dimethyloxetane + Methyl Cyclohexane and 3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	4.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of 3,3-Dimethyloxetane + Methyl Cyclohexane and 3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa: https://www.doi.org/10.1021/acs.jced.8b00966

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13401564&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume