1,3-Dichloro-2,2-dimethylpropane

Inchi: InChI=1S/C5H10Cl2/c1-5(2,3-6)4-7/h3-4H2,1-2H3
InchiKey: KTWNITKLQPCZSL-UHFFFAOYSA-N
Formula: C5H10Cl2
SMILES: CC(C)(CCl)CCl
Mol. weight [g/mol]: 141.04
CAS: 29559-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-29.80	kJ/mol	Joback Method
hf	-186.76	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	34.20	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.490		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	385.43	K	Joback Method
tc	579.04	K	Joback Method
tf	208.37	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.40	J/mol×K	385.43	Joback Method
cpg	187.56	J/mol×K	417.70	Joback Method
cpg	197.13	J/mol×K	449.97	Joback Method
cpg	206.13	J/mol×K	482.23	Joback Method
cpg	214.58	J/mol×K	514.50	Joback Method
cpg	222.52	J/mol×K	546.77	Joback Method
cpg	229.97	J/mol×K	579.04	Joback Method
dvisc	0.0077359	Pa×s	208.37	Joback Method
dvisc	0.0034334	Pa×s	237.88	Joback Method

dvisc	0.0018231	Pa×s	267.39	Joback Method
dvisc	0.0010979	Pa×s	296.90	Joback Method
dvisc	0.0007246	Pa×s	326.41	Joback Method
dvisc	0.0005124	Pa×s	355.92	Joback Method
dvisc	0.0003821	Pa×s	385.43	Joback Method
hfust	1.60	kJ/mol	262.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30293e+01
Coeff. B	-2.69860e+03
Coeff. C	-1.01893e+02
Temperature range (K), min.	313.69
Temperature range (K), max.	451.55

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29559555&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

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