Pentaerythrityl tetrachloride

Other names:	1,3-Dichloro-2,2-bis(chloromethyl) propane
	2,2-Bis(chloromethyl)-1,3-dichloropropane
	Methane, tetrakis(chloromethyl)-
	Pentaerythritol tetrachloride
	Propane, 1,3-dichloro-2,2-bis(chloromethyl)-
	Tetrakis(chloromethyl)methane
Inchi:	InChI=1S/C5H8Cl4/c6-1-5(2-7,3-8)4-9/h1-4H2
InchiKey:	KPZGRMZPZLOPBS-UHFFFAOYSA-N
Formula:	C5H8Cl4
SMILES:	ClCC(CCl)(CCl)CCl
Mol. weight [g/mol]:	209.93
CAS:	3228-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-53.66	kJ/mol	Joback Method
hf	-218.24	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	42.97	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.928		Crippen Method
mcvol	130.270	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
ss	257.48	J/mol×K	NIST Webbook
ss	257.48	J/mol×K	NIST Webbook
ss	240.62	J/mol×K	NIST Webbook
tb	460.29	K	Joback Method
tc	668.54	K	Joback Method
tf	268.21	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	225.21	J/mol×K	460.29	Joback Method
cpg	234.22	J/mol×K	495.00	Joback Method
cpg	270.30	J/mol×K	668.54	Joback Method
cpg	264.15	J/mol×K	633.83	Joback Method
cpg	257.50	J/mol×K	599.12	Joback Method
cpg	250.32	J/mol×K	564.42	Joback Method
cpg	242.58	J/mol×K	529.71	Joback Method
cps	198.49	J/mol×K	298.15	NIST Webbook
cps	198.49	J/mol×K	298.15	NIST Webbook
cps	186.94	J/mol×K	298.15	NIST Webbook
dvisc	0.0003739	Pa×s	460.29	Joback Method
dvisc	0.0006807	Pa×s	396.26	Joback Method
dvisc	0.0009941	Pa×s	364.25	Joback Method
dvisc	0.0015615	Pa×s	332.24	Joback Method
dvisc	0.0027007	Pa×s	300.22	Joback Method
dvisc	0.0053237	Pa×s	268.21	Joback Method
dvisc	0.0004933	Pa×s	428.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49623e+01
Coeff. B	-4.22683e+03
Coeff. C	-7.59800e+01
Temperature range (K), min.	364.01
Temperature range (K), max.	513.96

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3228997&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
pvap:	Vapor pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume