

P-xylene, 2,3,5,6-tetrachloro

Other names:	1,2,4,5-Tetrachloro-3,6-dimethylbenzene 2,3,5,6-tetrachloro-p-xylene Benzene, 1,2,4,5-tetrachloro-3,6-dimethyl-
Inchi:	InChI=1S/C8H6Cl4/c1-3-5(9)7(11)4(2)8(12)6(3)10/h1-2H3
InchiKey:	CTSQZGJZQUVGBQ-UHFFFAOYSA-N
Formula:	C8H6Cl4
SMILES:	Cc1c(Cl)c(Cl)c(C)c(Cl)c1Cl
Mol. weight [g/mol]:	243.94
CAS:	877-10-1

Physical Properties

Property code	Value	Unit	Source
chs	-3926.20	kJ/mol	NIST Webbook
chs	-3923.90 ± 0.59	kJ/mol	NIST Webbook
gf	33.02	kJ/mol	Joback Method
hf	-92.23	kJ/mol	Joback Method
hfs	-174.20	kJ/mol	NIST Webbook
hfs	-176.00	kJ/mol	NIST Webbook
hfus	25.36	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.917		Crippen Method
mcvol	148.780	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	583.74	K	Joback Method
tc	821.93	K	Joback Method
tf	370.00 ± 1.00	K	NIST Webbook
tf	521.00 ± 2.00	K	NIST Webbook
vc	0.572	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.52	J/mol×K	782.23	Joback Method

cpg	297.05	J/mol×K	742.54	Joback Method
cpg	290.12	J/mol×K	702.84	Joback Method
cpg	282.74	J/mol×K	663.14	Joback Method
cpg	274.90	J/mol×K	623.44	Joback Method
cpg	266.59	J/mol×K	583.74	Joback Method
cpg	309.55	J/mol×K	821.93	Joback Method
dvisc	0.0009119	Paxs	388.62	Joback Method
dvisc	0.0002454	Paxs	583.74	Joback Method
dvisc	0.0002863	Paxs	551.22	Joback Method
dvisc	0.0003406	Paxs	518.70	Joback Method
dvisc	0.0004147	Paxs	486.18	Joback Method
dvisc	0.0005193	Paxs	453.66	Joback Method
dvisc	0.0006733	Paxs	421.14	Joback Method
hfust	22.59	kJ/mol	368.20	NIST Webbook
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40947e+01
Coeff. B	-4.28666e+03
Coeff. C	-9.30910e+01
Temperature range (K), min.	403.56
Temperature range (K), max.	581.14

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=C877101&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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