Benzene, 1,2,3,5-tetrachloro-

Other names: 1,2,3,5-Tetrachlorobenzene
Inchi: InChI=1S/C6H2Cl4/c7-3-1-4(8)6(10)5(9)2-3/h1-2H
InchiKey: QZYNWJQFTJXIRN-UHFFFAOYSA-N
Formula: C6H2Cl4
SMILES: Clc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 215.89
CAS: 634-90-2

Physical Properties

Property code	Value	Unit	Source
chs	-2634.28 ± 0.48	kJ/mol	NIST Webbook
gf	35.44	kJ/mol	Joback Method
hf	-34.90	kJ/mol	NIST Webbook
hfus	20.96	kJ/mol	Joback Method
hsub	79.60 ± 0.30	kJ/mol	NIST Webbook
hsub	59.66	kJ/mol	NIST Webbook
hvap	60.70	kJ/mol	NIST Webbook
ie	9.26 ± 0.03	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
log10ws	-4.65		Aqueous Solubility Prediction Method
log10ws	-4.63		Estimated Solubility Method
logp	4.300		Crippen Method
mcvol	120.600	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1314.62		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1304.58		NIST Webbook
rinpol	1313.21		NIST Webbook
rinpol	1320.19		NIST Webbook
rinpol	1299.65		NIST Webbook

rinpol	1309.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1331.36		NIST Webbook
rinpol	228.00		NIST Webbook
rinpol	221.30		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1304.58		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	228.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1299.65		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1353.80		NIST Webbook
rinpol	1338.20		NIST Webbook
rinpol	1338.20		NIST Webbook
rinpol	1338.20		NIST Webbook
rinpol	1369.00		NIST Webbook
ripol	1790.60		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1813.33		NIST Webbook
ripol	1802.65		NIST Webbook
ripol	1782.97		NIST Webbook
ripol	1790.60		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1823.70		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1813.33		NIST Webbook
tb	519.20	K	NIST Webbook
tc	774.01	K	Joback Method
tf	326.65	K	Aqueous Solubility Prediction Method
tf	323.90 ± 0.20	K	NIST Webbook
tt	323.77 ± 0.01	K	NIST Webbook

vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.78	J/mol×K	569.02	Joback Method
cpg	198.52	J/mol×K	610.02	Joback Method
cpg	203.83	J/mol×K	651.01	Joback Method
cpg	217.36	J/mol×K	774.01	Joback Method
cpg	208.73	J/mol×K	692.01	Joback Method
cpg	213.23	J/mol×K	733.01	Joback Method
cpg	186.59	J/mol×K	528.02	Joback Method
dvisc	0.0003561	Pa×s	496.86	Joback Method
dvisc	0.0004323	Pa×s	465.69	Joback Method
dvisc	0.0005397	Pa×s	434.53	Joback Method
dvisc	0.0006972	Pa×s	403.37	Joback Method
dvisc	0.0009401	Pa×s	372.20	Joback Method
dvisc	0.0003001	Pa×s	528.02	Joback Method
dvisc	0.0013389	Pa×s	341.04	Joback Method
hfust	19.00	kJ/mol	323.90	NIST Webbook
hfust	18.32	kJ/mol	323.77	NIST Webbook
hfust	19.00	kJ/mol	323.90	NIST Webbook
hvapt	51.10	kJ/mol	425.00	NIST Webbook
sfust	56.60	J/mol×K	323.77	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38783e+01
Coeff. B	-4.01603e+03
Coeff. C	-8.55010e+01
Temperature range (K), min.	381.00
Temperature range (K), max.	554.29

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C634902&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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