

Benzene, 1,4-bis(trichloromethyl)-

Other names:	p-Xylene, «alpha», «alpha», «alpha», «alpha»', «alpha»', «alpha»'-hexachloro- «alpha», «alpha», «alpha», «alpha»', «alpha»', «alpha»'-Hexachloro-p-xylene «alpha», «alpha»'-Hexachloro-p-xylene «omega»-Hexachloro-p-xylene «omega», «omega»'-Hexachloro-p-xylene p-Bis(perchloromethyl)benzene p-Bis(trichloromethyl)benzene Bitriben Chloksil Chloxil Chloxyl Cloxil Hetol Hexachloroparaxylol Khloxil 1,4-Bis(trichloromethyl)benzene 1,4-Di(trichloromethyl)benzene p-Xylene hexachloride p-Xylene, «alpha», «alpha»'-hexachloro- Hexachloroxylyene Hexichol Khloksil 2,2-Hexachloro-p-xylene alpha,alpha,alpha,alpha',alpha',alpha'-Hexachloro-p-xylene NSC 41883
Inchi:	InChI=1S/C8H4Cl6/c9-7(10,11)5-1-2-6(4-3-5)8(12,13)14/h1-4H
InchiKey:	OTEKOJQFKOIXMU-UHFFFAOYSA-N
Formula:	C8H4Cl6
SMILES:	C1C(Cl)(Cl)C1ccc(C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]:	312.83
CAS:	68-36-0

Physical Properties

Property code	Value	Unit	Source
gf	53.36	kJ/mol	Joback Method
hf	-95.33	kJ/mol	Joback Method

hfus	20.48		kJ/mol	Joback Method
hvap	60.06		kJ/mol	Joback Method
log10ws	-5.48			Crippen Method
logp	5.340			Crippen Method
mcvol	173.260		ml/mol	McGowan Method
pc	2909.25		kPa	Joback Method
tb	632.22		K	Joback Method
tc	905.77		K	Joback Method
tf	403.22		K	Joback Method
vc	0.647		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.65	J/molxK	632.22	Joback Method
cpg	350.94	J/molxK	860.18	Joback Method
cpg	346.26	J/molxK	814.59	Joback Method
cpg	340.96	J/molxK	769.00	Joback Method
cpg	334.86	J/molxK	723.40	Joback Method
cpg	327.81	J/molxK	677.81	Joback Method
cpg	355.15	J/molxK	905.77	Joback Method
dvisc	0.0001718	Paxs	632.22	Joback Method
dvisc	0.0002227	Paxs	594.05	Joback Method
dvisc	0.0002992	Paxs	555.89	Joback Method
dvisc	0.0004199	Paxs	517.72	Joback Method
dvisc	0.0006219	Paxs	479.55	Joback Method
dvisc	0.0009858	Paxs	441.39	Joback Method
dvisc	0.0017051	Paxs	403.22	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C68360&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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