

Alpha,alpha,alpha,alpha',alpha',alpha'-2,5-octachlorobenzene

Other names:	Benzene, 1,4-dichloro-2,5-bis(trichloromethyl)-
Inchi:	InChI=1S/C8H2Cl8/c9-5-1-3(7(11,12)13)6(10)2-4(5)8(14,15)16/h1-2H
InchiKey:	RMXLFMXXVKFMFK-UHFFFAOYSA-N
Formula:	C8H2Cl8
SMILES:	Clc1cc(C(Cl)(Cl)Cl)c(Cl)cc1C(Cl)(Cl)Cl
Mol. weight [g/mol]:	381.73
CAS:	2142-29-2

Physical Properties

Property code	Value	Unit	Source
gf	10.24	kJ/mol	Joback Method
hf	-149.75	kJ/mol	Joback Method
hfus	28.10	kJ/mol	Joback Method
hvap	70.15	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.647		Crippen Method
mcvol	197.740	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
tb	717.04	K	Joback Method
tc	996.20	K	Joback Method
tf	488.10	K	Joback Method
vc	0.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.97	J/molxK	717.04	Joback Method
cpg	354.40	J/molxK	763.57	Joback Method
cpg	359.08	J/molxK	810.09	Joback Method
cpg	363.15	J/molxK	856.62	Joback Method
cpg	366.76	J/molxK	903.15	Joback Method
cpg	370.08	J/molxK	949.67	Joback Method
cpg	373.25	J/molxK	996.20	Joback Method
dvisc	0.0007579	Paxs	488.10	Joback Method

dvisc	0.0005004	Paxs	526.26	Joback Method
dvisc	0.0003494	Paxs	564.41	Joback Method
dvisc	0.0002554	Paxs	602.57	Joback Method
dvisc	0.0001937	Paxs	640.73	Joback Method
dvisc	0.0001516	Paxs	678.88	Joback Method
dvisc	0.0001218	Paxs	717.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2142292&Units=SI

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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