

1-Chloro-2,2-Bis(p-chlorophenyl)ethane

Other names:	Benzene, 1,1'-(2-chloroethylidene)bis-4-chloro- Ethane, 2-chloro-1,1-bis(p-chlorophenyl)- p,p'-DDMS DDM DDMS 1,1-Bis(p-chlorophenyl)-2-chloroethane Ethane, 2,2-bis(p-chlorophenyl)-1-chloro- 2,2-Bis(p-chlorophenyl)-1-monochloroethane
Inchi:	InChI=1S/C14H11Cl3/c15-9-14(10-1-5-12(16)6-2-10)11-3-7-13(17)8-4-11/h1-8,14H,9H2
InchiKey:	CHBOSHOWERDCMH-UHFFFAOYSA-N
Formula:	C14H11Cl3
SMILES:	C1CC(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	285.60
CAS:	2642-80-0

Physical Properties

Property code	Value	Unit	Source
gf	234.33	kJ/mol	Joback Method
hf	65.33	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	5.364		Crippen Method
mcvol	197.320	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	694.89	K	Joback Method
tc	950.58	K	Joback Method
tf	400.18	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.41	J/mol×K	694.89	Joback Method
cpg	462.99	J/mol×K	737.51	Joback Method
cpg	475.39	J/mol×K	780.12	Joback Method
cpg	486.70	J/mol×K	822.74	Joback Method
cpg	496.99	J/mol×K	865.35	Joback Method
cpg	506.35	J/mol×K	907.97	Joback Method
cpg	514.88	J/mol×K	950.58	Joback Method
dvisc	0.0013470	Paxs	400.18	Joback Method
dvisc	0.0007497	Paxs	449.30	Joback Method
dvisc	0.0004684	Paxs	498.42	Joback Method
dvisc	0.0003184	Paxs	547.54	Joback Method
dvisc	0.0002306	Paxs	596.65	Joback Method
dvisc	0.0001755	Paxs	645.77	Joback Method
dvisc	0.0001387	Paxs	694.89	Joback Method

Sources

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=C2642800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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

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