

Benzene, 1,1'-(2-chloroethylidene)bis[4-chloro-

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:	ClCC(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	285.60

Physical Properties

Property code	Value	Unit	Source
hf	51.85	kJ/mol	Cheméo Relay (1.0)
hfus	28.39	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-6.48		Cheméo Relay (1.0)
logp	5.364		Crippen Method
mcvol	197.320	ml/mol	McGowan Method
rinpol	2168.00		NIST Webbook
tb	622.35	K	Cheméo Relay (1.0)
tf	367.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.41	J/mol×K	694.89	Joback Method
cpg	514.88	J/mol×K	950.58	Joback Method
cpg	506.35	J/mol×K	907.97	Joback Method
cpg	496.99	J/mol×K	865.35	Joback Method

cpg	486.70	J/mol×K	822.74	Joback Method
cpg	475.39	J/mol×K	780.12	Joback Method
cpg	462.99	J/mol×K	737.51	Joback Method
dvisc	0.0003184	Pa×s	547.54	Joback Method
dvisc	0.0001387	Pa×s	694.89	Joback Method
dvisc	0.0001755	Pa×s	645.77	Joback Method
dvisc	0.0002306	Pa×s	596.65	Joback Method
dvisc	0.0013470	Pa×s	400.18	Joback Method
dvisc	0.0004684	Pa×s	498.42	Joback Method
dvisc	0.0007497	Pa×s	449.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642800&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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