

Benzene,(2,2-dichloroethyl)-

Inchi:	InChI=1S/C8H8Cl2/c9-8(10)6-7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey:	NGQTUWCDHLILAX-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	ClC(Cl)Cc1ccccc1
Mol. weight [g/mol]:	175.06
CAS:	4412-39-9

Physical Properties

Property code	Value	Unit	Source
gf	102.59	kJ/mol	Joback Method
hf	-8.68	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
ie	9.27	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	3.033		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
tb	483.54	K	Joback Method
tc	711.88	K	Joback Method
tf	251.18	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.00	J/molxK	483.54	Joback Method
cpg	238.86	J/molxK	521.60	Joback Method
cpg	249.88	J/molxK	559.65	Joback Method
cpg	260.12	J/molxK	597.71	Joback Method
cpg	269.60	J/molxK	635.77	Joback Method
cpg	278.37	J/molxK	673.83	Joback Method

cpg	286.48	J/mol×K	711.88	Joback Method
dvisc	0.0045517	Paxs	251.18	Joback Method
dvisc	0.0020744	Paxs	289.91	Joback Method
dvisc	0.0011378	Paxs	328.63	Joback Method
dvisc	0.0007083	Paxs	367.36	Joback Method
dvisc	0.0004826	Paxs	406.09	Joback Method
dvisc	0.0003516	Paxs	444.81	Joback Method
dvisc	0.0002695	Paxs	483.54	Joback Method

Sources

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=C4412399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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<https://www.chemeo.com/cid/63-684-3/Benzene-2-2-dichloroethyl.pdf>

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