

Cyclohexene, 1-chloro-4-(1-chloroethenyl)-

Other names:	Cyclohexene, 1-chloro-4-(1-chlorovinyl)- 1-Chloro-4-(«alpha»-chlorovinyl)cyclohexene
Inchi:	InChI=1S/C8H10Cl2/c1-6(9)7-2-4-8(10)5-3-7/h4,7H,1-3,5H2
InchiKey:	RRBHRPHCJASXKZ-UHFFFAOYSA-N
Formula:	C8H10Cl2
SMILES:	<chem>C=C(Cl)C1CC=C(Cl)CC1</chem>
Mol. weight [g/mol]:	177.07
CAS:	13547-06-3

Physical Properties

Property code	Value	Unit	Source
gf	116.69	kJ/mol	Joback Method
hf	-23.66	kJ/mol	Joback Method
hfus	14.95	kJ/mol	Joback Method
hvap	42.97	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.662		Crippen Method
mvol	128.600	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
tb	477.55	K	Joback Method
tc	705.31	K	Joback Method
tf	244.70	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.83	J/molxK	477.55	Joback Method
cpg	256.87	J/molxK	515.51	Joback Method
cpg	270.03	J/molxK	553.47	Joback Method
cpg	282.34	J/molxK	591.43	Joback Method
cpg	293.83	J/molxK	629.39	Joback Method

cpg	304.54	J/mol×K	667.35	Joback Method
cpg	314.50	J/mol×K	705.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13547063&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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
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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