

1-trans-2-trans-4-cis-5-Tetrachlorocyclohexane

Inchi:	InChI=1S/C6H8Cl4/c7-3-1-4(8)6(10)2-5(3)9/h3-6H,1-2H2/t3-,4+,5-,6+
InchiKey:	WCKYEVXZTBRMIY-FBXFSONDSA-N
Formula:	C6H8Cl4
SMILES:	C1C1CC(Cl)C(Cl)CC1Cl
Mol. weight [g/mol]:	221.94

Physical Properties

Property code	Value	Unit	Source
gf	-46.76	kJ/mol	Joback Method
hf	-236.83	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.210		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1361.00		NIST Webbook
rinpol	1362.00		NIST Webbook
tb	491.94	K	Joback Method
tc	724.89	K	Joback Method
tf	271.72	K	Joback Method
vc	0.497	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.99	J/molxK	491.94	Joback Method
cpg	261.75	J/molxK	530.76	Joback Method
cpg	274.71	J/molxK	569.59	Joback Method
cpg	286.88	J/molxK	608.41	Joback Method
cpg	298.26	J/molxK	647.24	Joback Method
cpg	308.87	J/molxK	686.06	Joback Method
cpg	318.71	J/molxK	724.89	Joback Method
dvisc	0.0020679	Paxs	271.72	Joback Method

dvisc	0.0013689	Paxs	308.42	Joback Method
dvisc	0.0009893	Paxs	345.13	Joback Method
dvisc	0.0007610	Paxs	381.83	Joback Method
dvisc	0.0006130	Paxs	418.53	Joback Method
dvisc	0.0005113	Paxs	455.24	Joback Method
dvisc	0.0004381	Paxs	491.94	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=R591552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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