

1,2,3,4,5-Pentachlorocyclo pentadiene

Inchi:	InChI=1S/C5HCl5/c6-1-2(7)4(9)5(10)3(1)8/h1H
InchiKey:	SPEJYXWMSKCTFT-UHFFFAOYSA-N
Formula:	C5HCl5
SMILES:	C1C=C(Cl)C(Cl)C(Cl)=C1Cl
Mol. weight [g/mol]:	238.33
CAS:	25329-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-10.48	kJ/mol	Joback Method
hf	-95.07	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.986		Crippen Method
mcvol	123.050	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	534.47	K	Joback Method
tc	778.23	K	Joback Method
tf	358.21	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.26	J/molxK	534.47	Joback Method
cpg	191.49	J/molxK	575.10	Joback Method
cpg	196.35	J/molxK	615.72	Joback Method
cpg	200.86	J/molxK	656.35	Joback Method
cpg	205.03	J/molxK	696.98	Joback Method
cpg	208.88	J/molxK	737.61	Joback Method
cpg	212.43	J/molxK	778.23	Joback Method
dvisc	0.0012522	Paxs	358.21	Joback Method
dvisc	0.0009813	Paxs	387.59	Joback Method

dvisc	0.0007959	Paxs	416.96	Joback Method
dvisc	0.0006635	Paxs	446.34	Joback Method
dvisc	0.0005657	Paxs	475.72	Joback Method
dvisc	0.0004914	Paxs	505.09	Joback Method
dvisc	0.0004335	Paxs	534.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C25329355&Units=SI

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

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