

Cyclopentadiene, chloro

Inchi:	InChI=1S/C5H5Cl/c6-5-3-1-2-4-5/h1,3-4H,2H2
InchiKey:	LJEOEPPSGGLCKY-UHFFFAOYSA-N
Formula:	C5H5Cl
SMILES:	C1C=CCC=C1
Mol. weight [g/mol]:	100.55

Physical Properties

Property code	Value	Unit	Source
gf	73.84	kJ/mol	Joback Method
hf	22.64	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	32.92	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.069		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
rinpola	716.00		NIST Webbook
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tb	374.48	K	Joback Method
tc	587.15	K	Joback Method
tf	205.21	K	Joback Method
vc	0.279	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.90	J/molxK	374.48	Joback Method
cpg	115.44	J/molxK	409.93	Joback Method
cpg	123.41	J/molxK	445.37	Joback Method
cpg	130.84	J/molxK	480.82	Joback Method
cpg	137.77	J/molxK	516.26	Joback Method
cpg	144.21	J/molxK	551.71	Joback Method
cpg	150.21	J/molxK	587.15	Joback Method
dvisc	0.0021001	Paxs	205.21	Joback Method

dvisc	0.0012593	Paxs	233.42	Joback Method
dvisc	0.0008432	Paxs	261.63	Joback Method
dvisc	0.0006104	Paxs	289.85	Joback Method
dvisc	0.0004680	Paxs	318.06	Joback Method
dvisc	0.0003746	Paxs	346.27	Joback Method
dvisc	0.0003101	Paxs	374.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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