

5-Chloro-3,4-dihydro-2H-pyran

Inchi:	InChI=1S/C5H7ClO/c6-5-2-1-3-7-4-5/h4H,1-3H2
InchiKey:	JEMCFUFHXLLFMO-UHFFFAOYSA-N
Formula:	C5H7ClO
SMILES:	C1C=COCCC1
Mol. weight [g/mol]:	118.56

Physical Properties

Property code	Value	Unit	Source
gf	-54.34	kJ/mol	Joback Method
hf	-173.30	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	37.31	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.877		Crippen Method
mcvol	84.260	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
tb	406.54	K	Joback Method
tc	626.46	K	Joback Method
tf	227.50	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.70	J/mol×K	406.54	Joback Method
cpg	188.43	J/mol×K	589.80	Joback Method
cpg	180.21	J/mol×K	553.15	Joback Method
cpg	171.44	J/mol×K	516.50	Joback Method
cpg	162.12	J/mol×K	479.85	Joback Method
cpg	152.21	J/mol×K	443.19	Joback Method
cpg	196.12	J/mol×K	626.46	Joback Method
dvisc	0.0003623	Pa×s	406.54	Joback Method

dvisc	0.0004763	Pa×s	376.70	Joback Method
dvisc	0.0006564	Pa×s	346.86	Joback Method
dvisc	0.0009609	Pa×s	317.02	Joback Method
dvisc	0.0015226	Pa×s	287.18	Joback Method
dvisc	0.0026844	Pa×s	257.34	Joback Method
dvisc	0.0054918	Pa×s	227.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132960&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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