

4-CHLOROTETRAHYDROPYRAN

Other names:	4-Chlorotetrahydropyran
Inchi:	InChI=1S/C5H9ClO/c6-5-1-3-7-4-2-5/h5H,1-4H2
InchiKey:	DHRSKOBIDIDMJZ-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	C1C1CCOCC1
Mol. weight [g/mol]:	120.58

Physical Properties

Property code	Value	Unit	Source
hf	-239.79	kJ/mol	Cheméo Relay (1.0)
hfus	12.72	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
logp	1.404		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
tb	425.91	K	Cheméo Relay (1.0)
tf	251.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.01	J/mol×K	397.73	Joback Method
cpg	166.79	J/mol×K	433.63	Joback Method
cpg	178.89	J/mol×K	469.52	Joback Method
cpg	190.34	J/mol×K	505.42	Joback Method
cpg	201.15	J/mol×K	541.32	Joback Method
cpg	211.34	J/mol×K	577.22	Joback Method
cpg	220.92	J/mol×K	613.11	Joback Method
dvisc	0.0073798	Pa×s	209.98	Joback Method
dvisc	0.0032986	Pa×s	241.27	Joback Method
dvisc	0.0017739	Pa×s	272.56	Joback Method
dvisc	0.0010839	Pa×s	303.86	Joback Method
dvisc	0.0007261	Pa×s	335.15	Joback Method
dvisc	0.0005209	Pa×s	366.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1768645&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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