Tetrahydrofurfuryl chloride

Other names:	Furan, 2-(chloromethyl)tetrahydro- 2-(Chloromethyl)tetrahydrofuran
Inchi:	InChI=1S/C5H9ClO/c6-4-5-2-1-3-7-5/h5H,1-4H2
InchiKey:	IVJLGIMHHWKRAN-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	ClCC1CCCO1
Mol. weight [g/mol]:	120.58
CAS:	3003-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-70.28	kJ/mol	Joback Method
hf	-233.79	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	35.88	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.404		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	423.70	K	NIST Webbook
tb	423.50 ± 0.50	K	NIST Webbook
tc	599.86	K	Joback Method
tf	213.50	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.99	J/mol×K	393.46	Joback Method
cpg	167.86	J/mol×K	427.86	Joback Method
cpg	179.09	J/mol×K	462.26	Joback Method

cpg	189.71	J/mol×K	496.66	Joback Method
cpg	199.73	J/mol×K	531.06	Joback Method
cpg	209.19	J/mol×K	565.46	Joback Method
cpg	218.09	J/mol×K	599.86	Joback Method
dvisc	0.0044638	Pa×s	213.50	Joback Method
dvisc	0.0023796	Pa×s	243.49	Joback Method
dvisc	0.0014562	Pa×s	273.49	Joback Method
dvisc	0.0009820	Pa×s	303.48	Joback Method
dvisc	0.0007108	Pa×s	333.47	Joback Method
dvisc	0.0005427	Pa×s	363.47	Joback Method
dvisc	0.0004318	Pa×s	393.46	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3003847&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
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