3-Chloro-tetrahydro-furan-2-carbonitrile

Inchi: InChI=1S/C5H6ClNO/c6-4-1-2-8-5(4)3-7/h4-5H,1-2H2
InchiKey: YTJXXPVBNLXGPI-UHFFFAOYSA-N
Formula: C5H6ClNO
SMILES: N#CC1OCCC1Cl
Mol. weight [g/mol]: 131.56

Physical Properties

Property code	Value	Unit	Source
gf	55.19	kJ/mol	Joback Method
hf	-89.25	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.906		Crippen Method
mcvol	89.940	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	995.00		NIST Webbook
tb	490.87	K	Joback Method
tc	720.56	K	Joback Method
tf	274.25	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.63	J/mol×K	490.87	Joback Method
cpg	192.69	J/mol×K	529.15	Joback Method
cpg	202.13	J/mol×K	567.43	Joback Method
cpg	210.98	J/mol×K	605.71	Joback Method
cpg	219.24	J/mol×K	644.00	Joback Method
cpg	226.94	J/mol×K	682.28	Joback Method
cpg	234.10	J/mol×K	720.56	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=R132797&Units=SI

Legend

cpg:	Ideal gas heat capacity
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