

3-chloro-2-Methoxy-tetrahydro-pyran

Inchi:	InChI=1S/C6H11ClO2/c1-8-6-5(7)3-2-4-9-6/h5-6H,2-4H2,1H3
InchiKey:	XYFHZQMPLJWQE-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	COC1OCCCC1Cl
Mol. weight [g/mol]:	150.60

Physical Properties

Property code	Value	Unit	Source
gf	-186.67	kJ/mol	Joback Method
hf	-413.15	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	40.38	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.377		Crippen Method
mcvol	108.520	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1050.00		NIST Webbook
tb	438.36	K	Joback Method
tc	649.66	K	Joback Method
tf	239.24	K	Joback Method
vc	0.392	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.82	J/molxK	438.36	Joback Method
cpg	230.83	J/molxK	473.58	Joback Method
cpg	244.25	J/molxK	508.79	Joback Method
cpg	257.06	J/molxK	544.01	Joback Method
cpg	269.26	J/molxK	579.23	Joback Method
cpg	280.85	J/molxK	614.44	Joback Method
cpg	291.83	J/molxK	649.66	Joback Method
dvisc	0.0035763	Paxs	239.24	Joback Method
dvisc	0.0018711	Paxs	272.43	Joback Method

dvisc	0.0011268	Paxs	305.61	Joback Method
dvisc	0.0007495	Paxs	338.80	Joback Method
dvisc	0.0005361	Paxs	371.99	Joback Method
dvisc	0.0004051	Paxs	405.17	Joback Method
dvisc	0.0003194	Paxs	438.36	Joback Method

Sources

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=R132940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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