

2H-Pyran, tetrahydro, 3-chloro-2-methoxy, # 2

Inchi: InChI=1S/C6H11ClO2/c1-8-6-5(7)3-2-4-9-6/h5-6H,2-4H2,1H3
InchiKey: XYYFHZQMPLJWQE-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	1060.00		NIST Webbook
tb	438.36	K	Joback Method
tc	649.66	K	Joback Method
tf	239.24	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0011268	Pa×s	305.61	Joback Method
dvisc	0.0007495	Pa×s	338.80	Joback Method
dvisc	0.0005361	Pa×s	371.99	Joback Method
dvisc	0.0004051	Pa×s	405.17	Joback Method
dvisc	0.0003194	Pa×s	438.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R91016&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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