2H-Pyran, tetrahydro-3-methyl-

Other names: 3-Methyltetrahydropyran
tetrahydro-3-methyl-2H-pyran
Inchi: InChI=1S/C6H12O/c1-6-3-2-4-7-5-6/h6H,2-5H2,1H3
InchiKey: UJQZTMFRMLEYQN-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1CCCOC1
Mol. weight [g/mol]: 100.16
CAS: 26093-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-62.03	kJ/mol	Joback Method
hf	-244.85	kJ/mol	Joback Method
hfus	11.11	kJ/mol	Joback Method
hvap	33.89	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.433		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	774.00		NIST Webbook
rinpol	774.00		NIST Webbook
tb	383.18	K	Joback Method
tc	588.02	K	Joback Method
tf	191.33	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.82	J/mol×K	383.18	Joback Method
cpg	178.37	J/mol×K	417.32	Joback Method
cpg	192.25	J/mol×K	451.46	Joback Method
cpg	205.45	J/mol×K	485.60	Joback Method
cpg	218.00	J/mol×K	519.74	Joback Method

cpg	229.91	J/mol×K	553.88	Joback Method
cpg	241.19	J/mol×K	588.02	Joback Method
dvisc	0.0082493	Pa×s	191.33	Joback Method
dvisc	0.0032943	Pa×s	223.30	Joback Method
dvisc	0.0016557	Pa×s	255.28	Joback Method
dvisc	0.0009699	Pa×s	287.25	Joback Method
dvisc	0.0006324	Pa×s	319.23	Joback Method
dvisc	0.0004457	Pa×s	351.21	Joback Method
dvisc	0.0003330	Pa×s	383.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	97.70	NIST Webbook

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=C26093630&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume