2,4-Dimethyltetrahydrofuran

Other names: furan, tetrahydro-2,4-dimethyl-
Inchi: InChI=1S/C6H12O/c1-5-3-6(2)7-4-5/h5-6H,3-4H2,1-2H3
InchiKey: QMGLMRPHOITLSN-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1COC(C)C1
Mol. weight [g/mol]: 100.16
CAS: 64265-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-57.64	kJ/mol	Joback Method
hf	-259.03	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	33.41	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	374.24	K	Joback Method
tc	569.86	K	Joback Method
tf	190.61	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.98	J/mol×K	374.24	Joback Method
cpg	229.04	J/mol×K	537.25	Joback Method
cpg	217.59	J/mol×K	504.65	Joback Method
cpg	205.56	J/mol×K	472.05	Joback Method
cpg	192.97	J/mol×K	439.45	Joback Method
cpg	179.78	J/mol×K	406.84	Joback Method
cpg	239.94	J/mol×K	569.86	Joback Method
dvisc	0.0003240	Pa×s	374.24	Joback Method

dvisc	0.0003887	Pa×s	343.63	Joback Method
dvisc	0.0004833	Pa×s	313.03	Joback Method
dvisc	0.0006300	Pa×s	282.43	Joback Method
dvisc	0.0008757	Pa×s	251.82	Joback Method
dvisc	0.0013336	Pa×s	221.22	Joback Method
dvisc	0.0023244	Pa×s	190.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37606e+01
Coeff. B	-3.07700e+03
Coeff. C	-4.42180e+01
Temperature range (K), min.	272.60
Temperature range (K), max.	408.40

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64265265&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume