Tetrahydrofuran, 2,2-dimethyl-

Other names: 2,2-Dimethyltetrahydrofuran
Inchi: InChI=1S/C6H12O/c1-6(2)4-3-5-7-6/h3-5H2,1-2H3
InchiKey: ZPDIRKNRUWXYLJ-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1(C)CCCO1
Mol. weight [g/mol]: 100.16
CAS: 1003-17-4

Physical Properties

Property code	Value	Unit	Source
affp	847.70	kJ/mol	NIST Webbook
basg	818.50	kJ/mol	NIST Webbook
gf	-55.42	kJ/mol	Joback Method
hf	-223.45	kJ/mol	Joback Method
hfus	6.91	kJ/mol	Joback Method
hvap	32.57	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.575		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	700.00		NIST Webbook
rinpol	700.00		NIST Webbook
tb	370.00 ± 4.00	K	NIST Webbook
tb	363.15 ± 2.00	K	NIST Webbook
tb	364.15 ± 1.00	K	NIST Webbook
tb	365.40 ± 0.05	K	NIST Webbook
tb	364.65 ± 1.50	K	NIST Webbook
tc	584.69	K	Joback Method
tf	158.69 ± 0.05	K	NIST Webbook
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	166.14	J/mol×K	379.15	Joback Method
cpg	180.73	J/mol×K	413.41	Joback Method
cpg	194.23	J/mol×K	447.66	Joback Method
cpg	206.73	J/mol×K	481.92	Joback Method
cpg	218.32	J/mol×K	516.18	Joback Method
cpg	229.09	J/mol×K	550.44	Joback Method
cpg	239.15	J/mol×K	584.69	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47025e+01
Coeff. B	-3.25146e+03
Coeff. C	-4.27170e+01
Temperature range (K), min.	268.28
Temperature range (K), max.	388.95

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003174&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume