Di-tert-Butyl ether

Other names:	(tert-C4H9)2O
	1,1'-OXYBIS(1,1-DIMETHYLETHANE)
	2,2'-OXYBIS-2-METHYL-PROPANE
	Propane, 2,2'-oxybis[2-methyl-
	tert-Butyl ether
Inchi:	InChI=1S/C8H18O/c1-7(2,3)9-8(4,5)6/h1-6H3
InchiKey:	AQEFLFZSWDEAIP-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)(C)OC(C)(C)C
Mol. weight [g/mol]:	130.23
CAS:	6163-66-2

Physical Properties

Property code	Value	Unit	Source
affp	887.40	kJ/mol	NIST Webbook
basg	860.00	kJ/mol	NIST Webbook
chl	-5318.30 ± 1.00	kJ/mol	NIST Webbook
chl	-5320.95	kJ/mol	NIST Webbook
chl	-5322.10 ± 0.61	kJ/mol	NIST Webbook
gf	-82.84	kJ/mol	Joback Method
hf	-361.90 ± 1.30	kJ/mol	NIST Webbook
hf	-362.00 ± 1.60	kJ/mol	NIST Webbook
hf	-361.10 ± 0.80	kJ/mol	NIST Webbook
hfl	-399.60 ± 1.20	kJ/mol	NIST Webbook
hfl	-402.00	kJ/mol	NIST Webbook
hfl	-398.45 ± 0.72	kJ/mol	NIST Webbook
hfus	2.84	kJ/mol	Joback Method
hvap	37.20	kJ/mol	NIST Webbook
hvap	37.70 ± 0.30	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	37.60 ± 0.10	kJ/mol	NIST Webbook
hvap	37.60 ± 0.90	kJ/mol	NIST Webbook
ie	8.88 ± 0.06	eV	NIST Webbook
ie	8.94 ± 0.01	eV	NIST Webbook
ie	8.81	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.600		Crippen Method

mcvol	129.450	ml/mol	McGowan Method
pc	2425.00 ± 150.00	kPa	NIST Webbook
pc	2420.00	kPa	KDB
rhoc	259.80 ± 11.98	kg/m3	NIST Webbook
tb	380.38	K	KDB
tb	379.90 ± 0.80	K	NIST Webbook
tc	555.00 ± 2.00	K	NIST Webbook
tc	550.00	K	KDB
tf	206.99	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.33	J/mol×K	584.50	Joback Method
cpg	331.31	J/mol×K	553.49	Joback Method
cpg	318.61	J/mol×K	522.47	Joback Method
cpg	305.18	J/mol×K	491.45	Joback Method
cpg	291.01	J/mol×K	460.43	Joback Method
cpg	276.06	J/mol×K	429.42	Joback Method
cpg	260.30	J/mol×K	398.40	Joback Method
cpl	276.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0019053	Pa×s	270.79	Joback Method
dvisc	0.0002653	Pa×s	398.40	Joback Method
dvisc	0.0127059	Pa×s	206.99	Joback Method
dvisc	0.0003818	Pa×s	366.50	Joback Method
dvisc	0.0005891	Pa×s	334.60	Joback Method
dvisc	0.0009959	Pa×s	302.69	Joback Method
dvisc	0.0043347	Pa×s	238.89	Joback Method
hvapt	37.30	kJ/mol	335.50	NIST Webbook
hvapt	31.60	kJ/mol	335.50	NIST Webbook
hvapt	38.70	kJ/mol	329.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.54392e+01
Coeff. B	-3.60333e+03
Coeff. C	-4.69010e+01
Temperature range (K), min.	284.72
Temperature range (K), max.	402.69

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1022.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6163662&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

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume