

Methanol, (tert-butyldioxy)-

Inchi:	InChI=1S/C6H14O2/c1-6(2,3)4-8-5-7/h7H,4-5H2,1-3H3
InchiKey:	XGHIDKRPCLIRGX-UHFFFAOYSA-N
Formula:	C5H12O3
SMILES:	CC(C)(C)COCO
Mol. weight [g/mol]:	120.15
CAS:	17742-78-8

Physical Properties

Property code	Value	Unit	Source
chl	-3201.00 ± 2.80	kJ/mol	NIST Webbook
gf	-239.34	kJ/mol	Joback Method
hf	-460.37	kJ/mol	Joback Method
hfl	-480.60 ± 2.80	kJ/mol	NIST Webbook
hfus	9.16	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.999		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	448.05	K	Joback Method
tc	618.94	K	Joback Method
tf	242.85	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.52	J/molxK	618.94	Joback Method
cpg	232.93	J/molxK	448.05	Joback Method
cpg	243.25	J/molxK	476.53	Joback Method
cpg	253.13	J/molxK	505.01	Joback Method
cpg	262.58	J/molxK	533.49	Joback Method
cpg	271.62	J/molxK	561.97	Joback Method
cpg	280.27	J/molxK	590.46	Joback Method

dvisc	0.0001995	Paxs	448.05	Joback Method
dvisc	0.0527584	Paxs	242.85	Joback Method
dvisc	0.0117321	Paxs	277.05	Joback Method
dvisc	0.0036303	Paxs	311.25	Joback Method
dvisc	0.0014170	Paxs	345.45	Joback Method
dvisc	0.0006553	Paxs	379.65	Joback Method
dvisc	0.0003442	Paxs	413.85	Joback Method
hvapt	59.60 ± 2.40	kJ/mol	290.00	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=C17742788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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