

1,3-Dioxolane, 2,4-dimethyl-

Other names:	1,3-Dioxolane, 2,4-dimethyl, cis 1,3-Dioxolane, 2,4-dimethyl, trans 2,4-dimethyl-1,3-dioxolane
Inchi:	InChI=1S/C5H10O2/c1-4-3-6-5(2)7-4/h4-5H,3H2,1-2H3
InchiKey:	ROSFUFIOLRQOON-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC1COC(C)O1
Mol. weight [g/mol]:	102.13
CAS:	3390-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-152.18	kJ/mol	Joback Method
hf	-370.39	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	35.69	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.768		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	674.00		NIST Webbook
tb	378.31	K	Joback Method
tc	576.19	K	Joback Method
tf	205.91	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.50	J/mol×K	576.19	Joback Method
cpg	169.66	J/mol×K	411.29	Joback Method
cpg	181.23	J/mol×K	444.27	Joback Method
cpg	192.30	J/mol×K	477.25	Joback Method
cpg	202.86	J/mol×K	510.23	Joback Method
cpg	212.92	J/mol×K	543.21	Joback Method
cpg	157.56	J/mol×K	378.31	Joback Method
dvisc	0.0004778	Pa×s	349.58	Joback Method
dvisc	0.0006014	Pa×s	320.84	Joback Method
dvisc	0.0007920	Pa×s	292.11	Joback Method
dvisc	0.0011077	Pa×s	263.38	Joback Method
dvisc	0.0016819	Pa×s	234.64	Joback Method
dvisc	0.0003931	Pa×s	378.31	Joback Method
dvisc	0.0028693	Pa×s	205.91	Joback Method
pvap	30.97	kPa	328.00	Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	44.43	kPa	338.00	Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	52.75	kPa	343.00	Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water

pvap	62.29	kPa	348.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	73.16	kPa	353.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	85.51	kPa	358.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	99.46	kPa	363.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	99.00	kPa	366.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water

pvap	25.62	kPa	323.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	21.04	kPa	318.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	17.17	kPa	313.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	13.90	kPa	308.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	11.17	kPa	303.00	Vapor-Liquid-Liquid Equilibrium (VLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water

pvap	8.89	kPa	298.00	Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water
pvap	37.21	kPa	333.00	Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor-Liquid-Liquid Equilibrium (VLLE) and Vapor Pressure Data for the Systems 2-Methyl-1,3-dioxolane (2MD) + Water and 2,4-Dimethyl-1,3-dioxolane (24DMD) + Water:	https://www.doi.org/10.1021/je025534p
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=C3390123&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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