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

Other names:	(.+/-.)-1,2-O-Isopropylideneglycerol
	(.+/-.)-Glycerol 1,2-acetonide
	(2,2-dimethyl-1,3-dioxolan-4-yl)methanol
	(4RS)-2,2-Dimethyl-1,3-dioxolane-4-methanol
	(RS)-Solketal
	1,2-Isopropylideneglycerin
	1,2-Isopropylideneglycerol
	1,2-O,O-Isopropylideneglycerin
	1,2-O-Isopropylideneglycerol
	2,2-Dimethyl-1,3-dioxolan-4-yl methanol
	2,2-Dimethyl-4-(hydroxymethyl)-1,3-dioxacyclopentane
	2,2-Dimethyl-4-hydroxymethyl-1,3-dioxolane
	2,2-Dimethyl-4-hydroxymethyldioxolane
	2,2-Dimethyl-4-oxymethyl-1,3-dioxolane
	2,2-Dimethyl-5-hydroxymethyl-1,3-dioxolane
	2,2-dimethyl-1,3-dioxolane-4-methanol
	2,3-(Isopropylidenedioxy)propanol
	2,3-Isopropylideneglycerol
	2,3-O-Isopropylideneglycerol
	4-Hydroxymethyl-2,2-dimethyl-1,3-dioxolane
	Acetone monoglycerol ketal
	Acetone, cyclic (hydroxymethyl)ethylene acetal
	Dioxolan
	GIE
	Glycerinisopropylidene ether
	Glycerol acetonide
	Glycerol dimethylketal
	Glycerol, 1,2-O-isopropylidene
	Glycerolacetone
	Isopropylidene glycerol
	NSC 59720
	Racemic solketal
	Solketal
	dl-«alpha»,«beta»-Isopropylideneglycerol
	«alpha»,«beta»-Isopropylideneglycerol
Inchi:	InChI=1S/C6H12O3/c1-6(2)8-4-5(3-7)9-6/h5,7H,3-4H2,1-2H3
InchiKey:	RNVYQYLELCKWAN-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CC1(C)OCC(CO)O1
Mol. weight [g/mol]:	132.16

CAS: 100-79-8

Physical Properties

Property code	Value	Unit	Source
dvisc	0.0100600	Pa×s	Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents
gf	-286.07	kJ/mol	Joback Method
hf	-528.02	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.130		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	461.70	K	NIST Webbook
tc	688.06	K	Joback Method
tf	301.90	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.77	J/mol×K	493.61	Joback Method
cpg	259.23	J/mol×K	526.02	Joback Method
cpg	269.97	J/mol×K	558.43	Joback Method
cpg	280.08	J/mol×K	590.84	Joback Method
cpg	289.63	J/mol×K	623.24	Joback Method
cpg	298.69	J/mol×K	655.65	Joback Method
cpg	307.33	J/mol×K	688.06	Joback Method
rhol	1069.30	kg/m3	298.15	Liquid-liquid equilibria for ternary mixtures of 2,2-dimethyl-1,3-dioxolane-4-methanol with n-heptane, toluene, ethanol and water

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
298.15	100.00	0.0100600

Reference *https://www.doi.org/10.1021/acs.jced.8b01042*

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities and Thermodynamic Properties of NH3 in Glycerin and its Derivatives:	https://www.doi.org/10.1021/acs.jced.8b01042
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100798&Units=SI
Vapor Liquid Equilibrium Data for Carbon Dioxide + (R/S)-1,2-Isopropylidene Glycerol (Solketal) + Oleic Acid Systems at High Pressure:	https://www.doi.org/10.1021/je401051d
Liquid-liquid equilibria for the system acetone + solketal + glycerol at 303.2 K and 323.2 K:	https://www.doi.org/10.1021/je500469a
Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents:	https://www.doi.org/10.1021/acs.jced.6b00399
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-liquid equilibria for ternary mixtures of 2,2-dimethyl-1,3-dioxolane-4-methanol with n-heptane, toluene, ethanol and water:	https://www.doi.org/10.1016/j.fluid.2015.07.016
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume