

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

Other names:	2,2-dimethyl-1,3-dioxolane Acetone, cyclic ethylene acetal acetone ethylene acetal
Inchi:	InChI=1S/C5H10O2/c1-5(2)6-3-4-7-5/h3-4H2,1-2H3
InchiKey:	SIJBDWPVNAYVGY-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC1(C)OCCO1
Mol. weight [g/mol]:	102.13
CAS:	2916-31-6

Physical Properties

Property code	Value	Unit	Source
chl	-2973.60 ± 2.90	kJ/mol	NIST Webbook
gf	-149.96	kJ/mol	Joback Method
hf	-334.81	kJ/mol	Joback Method
hfus	12.30	kJ/mol	Joback Method
hvap	34.85	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.769		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	365.70	K	NIST Webbook
tc	591.12	K	Joback Method
tf	234.05	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.48	J/mol×K	383.22	Joback Method
cpg	170.25	J/mol×K	417.87	Joback Method
cpg	182.02	J/mol×K	452.52	Joback Method

cpg	192.87	J/mol×K	487.17	Joback Method
cpg	202.91	J/mol×K	521.82	Joback Method
cpg	212.21	J/mol×K	556.47	Joback Method
cpg	220.87	J/mol×K	591.12	Joback Method
hvapt	41.10 ± 0.20	kJ/mol	298.00	NIST Webbook
rhoI	944.20	kg/m3	298.15	Liquid-liquid equilibria for multicomponent mixtures of 2,2-dimethyl-1,3-dioxolane with n-heptane, toluene, ethanol and water

Sources

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=C2916316&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibria for multicomponent mixtures of 2,2-dimethyl-1,3-dioxolane with n-heptane, toluene, ethanol and water:	https://www.doi.org/10.1016/j.fluid.2014.08.002

Legend

chl:	Standard liquid enthalpy of combustion
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
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
rhoI:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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