

1,3-Dioxolane, 4-methyl-

Other names:	4-Methyl-1,3-dioxolane
Inchi:	InChI=1S/C4H8O2/c1-4-2-5-3-6-4/h4H,2-3H2,1H3
InchiKey:	SBUOHGKIOVRDKY-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC1COCO1
Mol. weight [g/mol]:	88.11
CAS:	1072-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-152.89	kJ/mol	Joback Method
hf	-329.41	kJ/mol	Joback Method
hfus	16.01	kJ/mol	Joback Method
hvap	33.78	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	0.379		Crippen Method
mcvol	68.100	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
rinpol	636.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	634.00		NIST Webbook
tb	355.50 ± 2.50	K	NIST Webbook
tc	559.81	K	Joback Method
tf	198.88	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.57	J/mol×K	360.10	Joback Method
cpg	132.00	J/mol×K	393.39	Joback Method
cpg	141.94	J/mol×K	426.67	Joback Method
cpg	151.39	J/mol×K	459.96	Joback Method
cpg	160.37	J/mol×K	493.24	Joback Method
cpg	168.89	J/mol×K	526.53	Joback Method
cpg	176.96	J/mol×K	559.81	Joback Method
dvisc	0.0044930	Pa×s	198.88	Joback Method
dvisc	0.0023943	Pa×s	225.75	Joback Method
dvisc	0.0014587	Pa×s	252.62	Joback Method
dvisc	0.0009775	Pa×s	279.49	Joback Method
dvisc	0.0007028	Pa×s	306.36	Joback Method
dvisc	0.0005328	Pa×s	333.23	Joback Method
dvisc	0.0004210	Pa×s	360.10	Joback Method

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=C1072475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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