

1,3-Dioxan-5-ol

Other names:	1,3-Formalglycerol 5-Hydroxy-1,3-dioxane 5-Hydroxy-m-dioxane Glycerol formal m-Dioxan-5-ol
Inchi:	InChI=1S/C4H8O3/c5-4-1-6-3-7-2-4/h4-5H,1-3H2
InchiKey:	VCKSNYNVNSOWEE-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	OC1COCOC1
Mol. weight [g/mol]:	104.10
CAS:	4740-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-301.81	kJ/mol	Joback Method
hf	-487.80	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	0.56		Crippen Method
logp	-0.648		Crippen Method
mcvol	73.970	ml/mol	McGowan Method
pc	5713.21	kPa	Joback Method
tb	456.55	K	Joback Method
tc	655.33	K	Joback Method
tf	256.18	K	Joback Method
vc	0.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.17	J/mol×K	456.55	Joback Method
cpg	173.01	J/mol×K	489.68	Joback Method
cpg	182.37	J/mol×K	522.81	Joback Method
cpg	191.26	J/mol×K	555.94	Joback Method

cpg	199.67	J/mol×K	589.07	Joback Method
cpg	207.63	J/mol×K	622.20	Joback Method
cpg	215.14	J/mol×K	655.33	Joback Method
dvisc	0.0491988	Pa×s	256.18	Joback Method
dvisc	0.0128361	Pa×s	289.57	Joback Method
dvisc	0.0044216	Pa×s	322.97	Joback Method
dvisc	0.0018599	Pa×s	356.37	Joback Method
dvisc	0.0009075	Pa×s	389.76	Joback Method
dvisc	0.0004959	Pa×s	423.15	Joback Method
dvisc	0.0002960	Pa×s	456.55	Joback Method

Sources

Solubilities and Thermodynamic Properties of NH₃ in Glycerin and its Derivatives:

<https://www.doi.org/10.1021/acs.jced.8b01042>

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4740787&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents:

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1021/acs.jced.6b00399>

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

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