1,4-Dioxane-2,5-dione

Other names:	1,4-dioxane, 2,5-dioxo-
	2,5-dioxo-1,4-dioxane
	Acetic acid, hydroxy-, bimol. cyclic ester
	Glycollide
	glycolide
	p-Dioxane-2,5-dione
Inchi:	InChI=1S/C4H4O4/c5-3-1-7-4(6)2-8-3/h1-2H2
InchiKey:	RKDVKSZUMVYZHH-UHFFFAOYSA-N
Formula:	C4H4O4
SMILES:	O=C1COC(=O)CO1
Mol. weight [g/mol]:	116.07
CAS:	502-97-6

Physical Properties

Property code	Value	Unit	Source
chs	-1445.40 ± 0.59	kJ/mol	NIST Webbook
chs	-1445.40 ± 0.60	kJ/mol	NIST Webbook
chs	-1441.80 ± 0.60	kJ/mol	NIST Webbook
gf	-402.46	kJ/mol	Joback Method
hf	-612.00 ± 1.40	kJ/mol	NIST Webbook
hf	-615.60	kJ/mol	NIST Webbook
hf	-611.90	kJ/mol	NIST Webbook
hfs	-700.30 ± 0.60	kJ/mol	NIST Webbook
hfs	-700.40 ± 0.59	kJ/mol	NIST Webbook
hfs	-704.00 ± 0.60	kJ/mol	NIST Webbook
hfus	11.86	kJ/mol	Joback Method
hsub	88.40 ± 0.80	kJ/mol	NIST Webbook
hsub	88.40	kJ/mol	NIST Webbook
hvap	42.75	kJ/mol	Joback Method
log10ws	0.88		Crippen Method
logp	-0.914		Crippen Method
mcvol	71.240	ml/mol	McGowan Method
pc	5809.41	kPa	Joback Method
ss	157.20	J/mol×K	NIST Webbook
ss	157.20	J/mol×K	NIST Webbook
ss	157.23	J/mol×K	NIST Webbook
ss	157.20	J/mol×K	NIST Webbook

tb	504.68	K	Joback Method
tc	755.81	K	Joback Method
tf	336.04	K	Joback Method
tt	356.20 ± 0.20	K	NIST Webbook
tt	356.20 ± 0.10	K	NIST Webbook
tt	317.51	K	Estimation and confirmation of the thermodynamic stability relationships of the enantiotropic polymorphs of glycolide
tt	316.55	K	Thermodynamic properties of enantiotropic polymorphs of glycolide
vc	0.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.63	J/mol×K	755.81	Joback Method
cpg	166.76	J/mol×K	546.54	Joback Method
cpg	176.68	J/mol×K	588.39	Joback Method
cpg	186.20	J/mol×K	630.25	Joback Method
cpg	195.24	J/mol×K	672.10	Joback Method
cpg	203.75	J/mol×K	713.96	Joback Method
cpg	156.52	J/mol×K	504.68	Joback Method
cps	133.30	J/mol×K	298.15	NIST Webbook
cps	133.28	J/mol×K	298.15	NIST Webbook
cps	133.30	J/mol×K	298.15	NIST Webbook
cps	133.20	J/mol×K	298.15	NIST Webbook
hfust	14.80	kJ/mol	356.20	NIST Webbook
hfust	1.81	kJ/mol	312.10	NIST Webbook
hfust	14.80	kJ/mol	356.20	NIST Webbook
hvapt	50.40	kJ/mol	444.50	NIST Webbook
sfust	5.82	J/mol×K	312.10	NIST Webbook
sfust	41.55	J/mol×K	356.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C502976&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of enantiotropic polymorphs of glycolide:	https://www.doi.org/10.1016/j.jct.2017.03.011
Estimation and confirmation of the thermodynamic stability relationships of the enantiotropic polymorphs of glycolide:	https://www.doi.org/10.1016/j.jct.2017.10.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume