1,4-Dioxane-2,6-dione

Other names:	Diglycolic anhydride
	Acetic acid, oxydi-, cyclic anhydride
	p-Dioxane-2,6-dione
	Acetic acid, 2,2'-oxybis-, cyclic anhydride
	Diglycolic acid anhydride
	Oxydiacetic anhydride
Inchi:	InChI=1S/C4H4O4/c5-3-1-7-2-4(6)8-3/h1-2H2
InchiKey:	PIYNUZCGMLCXKJ-UHFFFAOYSA-N
Formula:	C4H4O4
SMILES:	O=C1COCC(=O)O1
Mol. weight [g/mol]:	116.07
CAS:	4480-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-402.46	kJ/mol	Joback Method
hf	-590.63	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
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
tb	513.70	K	NIST Webbook
tc	755.81	K	Joback Method
tf	336.04	K	Joback Method
vc	0.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.52	J/mol×K	504.68	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	211.63	J/mol×K	755.81	Joback Method
hsubt	84.20 ± 1.10	kJ/mol	342.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C4480835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hsubt:	Enthalpy of sublimation at a given temperature
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