P-dioxan-2-one

Other names:	1,4-Dioxan-2-one
	p-dioxanone
Inchi:	InChI=1S/C4H6O3/c5-4-3-6-1-2-7-4/h1-3H2
InchiKey:	VPVXHAANQNHFSF-UHFFFAOYSA-N
Formula:	C4H6O3
SMILES:	O=C1COCCO1
Mol. weight [g/mol]:	102.09
CAS:	3041-16-5

Physical Properties

Property code	Value	Unit	Source
gf	-279.87	kJ/mol	Joback Method
hf	-452.93	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Solubility, Density, and Metastable Zone Width of the (1,4-Dioxan-2-one + Ethyl Acetate) System
hfus	15.70	kJ/mol	Solubility of Organic Systems Containing 1,4-Dioxan-2-one
hvap	38.50	kJ/mol	Joback Method
log10ws	0.66		Crippen Method
logp	-0.440		Crippen Method
mcvol	69.670	ml/mol	McGowan Method
pc	5511.44	kPa	Joback Method
tb	436.86	K	Joback Method
tc	668.81	K	Joback Method
tf	267.82	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.39	J/mol×K	436.86	Joback Method
cpg	149.82	J/mol×K	475.52	Joback Method

cpg	159.83	J/mol×K	514.18	Joback Method
cpg	169.41	J/mol×K	552.84	Joback Method
cpg	178.53	J/mol×K	591.50	Joback Method
cpg	187.19	J/mol×K	630.16	Joback Method
cpg	195.35	J/mol×K	668.81	Joback Method
hfust	16.14	kJ/mol	301.70	NIST Webbook
hfust	16.14	kJ/mol	301.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3041165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility, Density, and Metastable Zone Width of the (1,4-Dioxan-2-one + Ethyl Acetate) System:	https://www.doi.org/10.1021/je050149w
Solubility of Organic Systems Containing 1,4-Dioxan-2-one:	https://www.doi.org/10.1021/je050406x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion 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

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