5,5-Dimethyl-1,3-dioxan-2-one

Other names:	5,5-Dimethyl-1,3-diox-2-one
	Neopentylene carbonate
	1,3-Dioxan-2-one, 5,5-dimethyl-
	Carbonic acid, cyclic 2,2-dimethyltrimethylene ester
Inchi:	InChI=1S/C6H10O3/c1-6(2)3-8-5(7)9-4-6/h3-4H2,1-2H3
InchiKey:	JRFXQKZEGILCCO-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC1(C)COC(=O)OC1
Mol. weight [g/mol]:	130.14
CAS:	3592-12-9

Physical Properties

Property code	Value	Unit	Source
chs	-3119.30 ± 1.20	kJ/mol	NIST Webbook
gf	-276.23	kJ/mol	Joback Method
hf	-499.31	kJ/mol	Joback Method
hfs	-670.90 ± 1.20	kJ/mol	NIST Webbook
hfus	12.30	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	1.179		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	478.19	K	Joback Method
tc	712.86	K	Joback Method
tf	310.02	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.54	J/mol×K	478.19	Joback Method
cpg	234.18	J/mol×K	517.30	Joback Method
cpg	246.97	J/mol×K	556.41	Joback Method

cpg	259.00	J/mol×K	595.52	Joback Method
cpg	270.35	J/mol×K	634.64	Joback Method
cpg	281.12	J/mol×K	673.75	Joback Method
cpg	291.38	J/mol×K	712.86	Joback Method
hfust	5.62	kJ/mol	387.20	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=C3592129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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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