1,3-Dioxane, 2,2-dimethyl-

Other names: 2,2-Dimethyl-1,3-dioxane
Inchi: InChI=1S/C6H12O2/c1-6(2)7-4-3-5-8-6/h3-5H2,1-2H3
InchiKey: RPLSBADGISFNSI-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC1(C)OCCCO1
Mol. weight [g/mol]: 116.16
CAS: 695-30-7

Physical Properties

Property code	Value	Unit	Source
chl	-3607.20 ± 2.00	kJ/mol	NIST Webbook
gf	-153.64	kJ/mol	Joback Method
hf	-361.61	kJ/mol	Joback Method
hfl	-468.90 ± 2.00	kJ/mol	NIST Webbook
hfus	12.79	kJ/mol	Joback Method
hvap	37.25	kJ/mol	Joback Method
ie	9.84	eV	NIST Webbook
log10ws	-1.01		Crippen Method
logp	1.159		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	796.00		NIST Webbook
tb	397.65 ± 1.50	K	NIST Webbook
tc	625.18	K	Joback Method
tf	241.80	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.00	J/mol×K	410.37	Joback Method
cpg	208.82	J/mol×K	446.17	Joback Method
cpg	222.56	J/mol×K	481.97	Joback Method

cpg	235.32	J/mol×K	517.77	Joback Method
cpg	247.20	J/mol×K	553.57	Joback Method
cpg	258.29	J/mol×K	589.38	Joback Method
cpg	268.70	J/mol×K	625.18	Joback Method
hfust	12.10	kJ/mol	229.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C695307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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