2-(1-Hydroxy-1-methylethyl-2-methyl-1,3-dioxane

Inchi: InChI=1S/C8H16O3/c1-7(2,9)8(3)10-5-4-6-11-8/h9H,4-6H2,1-3H3
InchiKey: JTBUTVUSECYYFH-UHFFFAOYSA-N
Formula: C8H16O3
SMILES: CC(C)(O)C1(C)OCCCO1
Mol. weight [g/mol]: 160.21
CAS: 39239-96-8

Physical Properties

Property code	Value	Unit	Source
chl	-4726.10 ± 6.20	kJ/mol	NIST Webbook
gf	-270.78	kJ/mol	Joback Method
hf	-642.00 ± 14.00	kJ/mol	NIST Webbook
hfl	-709.00 ± 12.00	kJ/mol	NIST Webbook
hfus	14.64	kJ/mol	Joback Method
hvap	67.40 ± 2.00	kJ/mol	NIST Webbook
hvap	67.00	kJ/mol	NIST Webbook
log10ws	-1.22		Crippen Method
logp	0.910		Crippen Method
mcvol	130.330	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	545.08	K	Joback Method
tc	753.48	K	Joback Method
tf	327.58	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.82	J/mol×K	545.08	Joback Method
cpg	353.24	J/mol×K	579.81	Joback Method
cpg	366.68	J/mol×K	614.55	Joback Method
cpg	379.26	J/mol×K	649.28	Joback Method
cpg	391.09	J/mol×K	684.01	Joback Method
cpg	402.28	J/mol×K	718.75	Joback Method

cpg	412.94	J/mol×K	753.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39239968&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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