1,3-Dioxane, 2,2-dimethyl-5-hydroxy-

Inchi: InChI=1S/C6H12O3/c1-6(2)8-3-5(7)4-9-6/h5,7H,3-4H2,1-2H3
InchiKey: CGNOMSJAJQUXAT-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CC1(C)OCC(O)CO1
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
gf	-298.17	kJ/mol	Joback Method
hf	-534.18	kJ/mol	Joback Method
hfus	17.95	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.130		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
tb	497.88	K	Joback Method
tc	699.56	K	Joback Method
tf	298.38	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.23	J/mol×K	497.88	Joback Method
cpg	259.49	J/mol×K	531.49	Joback Method
cpg	270.98	J/mol×K	565.11	Joback Method
cpg	281.80	J/mol×K	598.72	Joback Method
cpg	292.02	J/mol×K	632.34	Joback Method
cpg	301.71	J/mol×K	665.95	Joback Method
cpg	310.94	J/mol×K	699.56	Joback Method

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=U381756&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume