cis-2,2,4,6-Tetramethyl-1,3-dioxane

Inchi: InChI=1S/C8H16O2/c1-6-5-7(2)10-8(3,4)9-6/h6-7H,5H2,1-4H3/t6-,7+
InchiKey: GPKRWHGIASNHBE-KNVOCYPGSA-N
Formula: C8H16O2
SMILES: CC1CC(C)OC(C)(C)O1
Mol. weight [g/mol]: 144.21
CAS: 17227-17-7

Physical Properties

Property code	Value	Unit	Source
chl	-4895.40 ± 3.40	kJ/mol	NIST Webbook
gf	-152.22	kJ/mol	Joback Method
hf	-498.00 ± 3.00	kJ/mol	NIST Webbook
hf	-496.40 ± 3.50	kJ/mol	NIST Webbook
hfl	-539.40 ± 3.40	kJ/mol	NIST Webbook
hfus	20.11	kJ/mol	Joback Method
hvap	43.00 ± 1.00	kJ/mol	NIST Webbook
hvap	42.30 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.936		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	446.79	K	Joback Method
tc	655.64	K	Joback Method
tf	255.86	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.84	J/mol×K	446.79	Joback Method
cpg	295.30	J/mol×K	481.60	Joback Method
cpg	311.72	J/mol×K	516.41	Joback Method
cpg	327.19	J/mol×K	551.22	Joback Method
cpg	341.78	J/mol×K	586.02	Joback Method

cpg	355.58	J/mol×K	620.83	Joback Method
cpg	368.66	J/mol×K	655.64	Joback Method

Sources

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=C17227177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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