cis-2,5-Diisopropyl-1,3-dioxane

Inchi: InChI=1S/C10H20O2/c1-7(2)9-5-11-10(8(3)4)12-6-9/h7-10H,5-6H2,1-4H3/t9-,10+
InchiKey: YAISJNQHUBKIPN-AOOOYVTPSA-N
Formula: C10H20O2
SMILES: CC(C)C1COC(C(C)C)OC1
Mol. weight [g/mol]: 172.26
CAS: 25925-00-2

Physical Properties

Property code	Value	Unit	Source
chl	-6169.00 ± 18.00	kJ/mol	NIST Webbook
gf	-127.06	kJ/mol	Joback Method
hf	-490.31	kJ/mol	Joback Method
hfl	-625.00 ± 18.00	kJ/mol	NIST Webbook
hfus	23.47	kJ/mol	Joback Method
hvap	46.22	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.288		Crippen Method
mcvol	152.640	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	496.10	K	Joback Method
tc	700.34	K	Joback Method
tf	228.74	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.52	J/mol×K	496.10	Joback Method
cpg	388.02	J/mol×K	530.14	Joback Method
cpg	406.58	J/mol×K	564.18	Joback Method
cpg	424.19	J/mol×K	598.22	Joback Method
cpg	440.89	J/mol×K	632.26	Joback Method
cpg	456.68	J/mol×K	666.30	Joback Method
cpg	471.58	J/mol×K	700.34	Joback Method

dvisc	0.0134801	Pa×s	228.74	Joback Method
dvisc	0.0041346	Pa×s	273.30	Joback Method
dvisc	0.0017664	Pa×s	317.86	Joback Method
dvisc	0.0009302	Pa×s	362.42	Joback Method
dvisc	0.0005637	Pa×s	406.98	Joback Method
dvisc	0.0003771	Pa×s	451.54	Joback Method
dvisc	0.0002711	Pa×s	496.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25925002&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
dvisc:	Dynamic viscosity
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

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