1,3-Dioxane, 2,4-diisopropyl-5,5-dimethyl-

Other names: 2,4-diisopropyl-5,5-dimethyl-1,3-dioxane
Inchi: InChI=1S/C12H24O2/c1-8(2)10-12(5,6)7-13-11(14-10)9(3)4/h8-11H,7H2,1-6H3
InchiKey: SVYIRYSQKUXBPY-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CC(C)C1OCC(C)(C)C(C(C)C)O1
Mol. weight [g/mol]: 200.32
CAS: 3494-76-6

Physical Properties

Property code	Value	Unit	Source
gf	-123.42	kJ/mol	Joback Method
hf	-536.69	kJ/mol	Joback Method
hfus	23.43	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.066		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
tb	537.43	K	Joback Method
tc	743.73	K	Joback Method
tf	270.94	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.29	J/mol×K	537.43	Joback Method
cpg	488.45	J/mol×K	571.81	Joback Method
cpg	508.46	J/mol×K	606.20	Joback Method
cpg	527.42	J/mol×K	640.58	Joback Method
cpg	545.40	J/mol×K	674.96	Joback Method
cpg	562.50	J/mol×K	709.34	Joback Method
cpg	578.81	J/mol×K	743.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3494766&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume