5,5-Dimethyl-2-isopropyl-1,3-dioxane

Other names: 2-Isopropyl-5,5-Dimethyl-1,3-dioxane
Inchi: InChI=1S/C9H18O2/c1-7(2)8-10-5-9(3,4)6-11-8/h7-8H,5-6H2,1-4H3
InchiKey: AWSZUOKHFRWQFK-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CC(C)C1OCC(C)(C)CO1
Mol. weight [g/mol]: 158.24
CAS: 7651-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-138.53	kJ/mol	Joback Method
hf	-449.15	kJ/mol	Joback Method
hfus	18.11	kJ/mol	Joback Method
hvap	43.23	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	2.042		Crippen Method
mcvol	138.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	473.90	K	Joback Method
tc	685.12	K	Joback Method
tf	256.37	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.21	J/mol×K	473.90	Joback Method
cpg	340.62	J/mol×K	509.10	Joback Method
cpg	357.91	J/mol×K	544.31	Joback Method
cpg	374.17	J/mol×K	579.51	Joback Method
cpg	389.49	J/mol×K	614.71	Joback Method
cpg	403.96	J/mol×K	649.92	Joback Method
cpg	417.69	J/mol×K	685.12	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=C7651505&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume