4,4,6-Trimethyl-2-vinyl-1,3-dioxane

Other names: 1,3-Dioxane, 4,4,6-trimethyl-2-vinyl-
2-Vinyl-4,4,6-trimethyl-1,3-dioxane
Inchi: InChI=1S/C9H16O2/c1-5-8-10-7(2)6-9(3,4)11-8/h5,7-8H,1,6H2,2-4H3
InchiKey: XLVQNXPLYGVRKU-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C=CC1OC(C)CC(C)(C)O1
Mol. weight [g/mol]: 156.22
CAS: 22634-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-55.96	kJ/mol	Joback Method
hf	-338.78	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	42.64	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.103		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
tb	466.35	K	Joback Method
tc	677.06	K	Joback Method
tf	265.37	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.01	J/mol×K	466.35	Joback Method
cpg	322.75	J/mol×K	501.47	Joback Method
cpg	339.40	J/mol×K	536.59	Joback Method
cpg	355.05	J/mol×K	571.71	Joback Method
cpg	369.80	J/mol×K	606.82	Joback Method
cpg	383.72	J/mol×K	641.94	Joback Method
cpg	396.92	J/mol×K	677.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22634895&Units=SI

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