M-dioxane, 2-propenyl-4-isopropyl-5,5-dimethyl-

Inchi: InChI=1S/C12H22O2/c1-6-7-10-13-8-12(4,5)11(14-10)9(2)3/h6-7,9-11H,8H2,1-5H3/b7-6
InchiKey: XYVOPPDFTDZQRJ-VOTSOKGWSA-N
Formula: C12H22O2
SMILES: CC=CC1OCC(C)(C)C(C(C)C)O1
Mol. weight [g/mol]: 198.30
CAS: 116373-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-40.76	kJ/mol	Joback Method
hf	-414.19	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	49.56	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.986		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
tb	542.03	K	Joback Method
tc	753.12	K	Joback Method
tf	280.86	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.27	J/mol×K	542.03	Joback Method
cpg	469.65	J/mol×K	577.21	Joback Method
cpg	488.85	J/mol×K	612.39	Joback Method
cpg	506.98	J/mol×K	647.58	Joback Method
cpg	524.14	J/mol×K	682.76	Joback Method
cpg	540.44	J/mol×K	717.94	Joback Method
cpg	555.99	J/mol×K	753.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373718&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

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