Methyl isopropenyl ketone dimer

Inchi: InChI=1S/C10H16O2/c1-7(11)9(3)5-10(4,6-9)8(2)12/h5-6H2,1-4H3
InchiKey: VZJNDGWZRZNTTK-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC(=O)C1(C)CC(C)(C(C)=O)C1
Mol. weight [g/mol]: 168.23
CAS: 116373-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-194.56	kJ/mol	Joback Method
hf	-398.11	kJ/mol	Joback Method
hfus	9.36	kJ/mol	Joback Method
hvap	48.82	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.971		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	542.76	K	Joback Method
tc	760.90	K	Joback Method
tf	360.30	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.94	J/mol×K	542.76	Joback Method
cpg	365.97	J/mol×K	579.12	Joback Method
cpg	379.93	J/mol×K	615.47	Joback Method
cpg	393.04	J/mol×K	651.83	Joback Method
cpg	405.50	J/mol×K	688.19	Joback Method
cpg	417.52	J/mol×K	724.54	Joback Method
cpg	429.31	J/mol×K	760.90	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=C116373456&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