2,6,6-trimethyl-2-vinyltetrahydropyran-3-one

Inchi: InChI=1S/C10H16O2/c1-5-10(4)8(11)6-7-9(2,3)12-10/h5H,1,6-7H2,2-4H3
InchiKey: CISPSXPKLLDNCN-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: C=CC1(C)OC(C)(C)CCC1=O
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-81.79	kJ/mol	Joback Method
hf	-329.54	kJ/mol	Joback Method
hfus	8.17	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.089		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
ripol	1478.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	535.01	K	Joback Method
tc	770.10	K	Joback Method
tf	346.43	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.47	J/mol×K	535.01	Joback Method
cpg	369.18	J/mol×K	574.19	Joback Method
cpg	385.73	J/mol×K	613.37	Joback Method
cpg	401.35	J/mol×K	652.56	Joback Method
cpg	416.23	J/mol×K	691.74	Joback Method

cpg	430.58	J/mol×K	730.92	Joback Method
cpg	444.63	J/mol×K	770.10	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=R303330&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume