2,2,6-Trimethyl-6-vinyl dihydropyran-3-one

Inchi: InChI=1S/C11H16O/c1-5-11(4)7-6-9(12)10(2,3)8-11/h5-7H,1,8H2,2-4H3
InchiKey: POKLXQZSXUILKQ-UHFFFAOYSA-N
Formula: C11H16O
SMILES: C=CC1(C)C=CC(=O)C(C)(C)C1
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	42.71	kJ/mol	Joback Method
hf	-160.40	kJ/mol	Joback Method
hfus	4.01	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.734		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1089.00		NIST Webbook
tb	530.10	K	Joback Method
tc	765.67	K	Joback Method
tf	331.89	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.05	J/mol×K	530.10	Joback Method
cpg	367.09	J/mol×K	569.36	Joback Method
cpg	383.90	J/mol×K	608.62	Joback Method
cpg	399.70	J/mol×K	647.88	Joback Method
cpg	414.73	J/mol×K	687.14	Joback Method
cpg	429.19	J/mol×K	726.41	Joback Method
cpg	443.30	J/mol×K	765.67	Joback Method

Sources

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=R227251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume