2H-Pyran-2-one, 5,6-dihydro-4,6,6-trimethyl-

Inchi: InChI=1S/C8H12O2/c1-6-4-7(9)10-8(2,3)5-6/h4H,5H2,1-3H3
InchiKey: ZSQHRLJAKWRVJQ-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CC1=CC(=O)OC(C)(C)C1
Mol. weight [g/mol]: 140.18
CAS: 6970-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-152.94	kJ/mol	Joback Method
hf	-362.28	kJ/mol	Joback Method
hfus	10.33	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
ripol	1905.00		NIST Webbook
tb	501.14	K	Joback Method
tc	733.34	K	Joback Method
tf	298.60 ± 0.60	K	NIST Webbook
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.14	J/mol×K	501.14	Joback Method
cpg	275.78	J/mol×K	539.84	Joback Method
cpg	289.56	J/mol×K	578.54	Joback Method
cpg	302.58	J/mol×K	617.24	Joback Method
cpg	314.93	J/mol×K	655.94	Joback Method
cpg	326.69	J/mol×K	694.64	Joback Method
cpg	337.94	J/mol×K	733.34	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=C6970565&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