5-hydroxy-4,6,6-trimethyl-4-cyclohexene-1,3-dion

Inchi: InChI=1S/C9H12O3/c1-5-6(10)4-7(11)9(2,3)8(5)12/h12H,4H2,1-3H3
InchiKey: APMOMMBTSMGEHZ-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: CC1=C(O)C(C)(C)C(=O)CC1=O
Mol. weight [g/mol]: 168.19

Physical Properties

Property code	Value	Unit	Source
gf	-327.44	kJ/mol	Joback Method
hf	-552.32	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.386		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
tb	662.05	K	Joback Method
tc	887.72	K	Joback Method
tf	445.53	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.06	J/mol×K	662.05	Joback Method
cpg	366.06	J/mol×K	699.66	Joback Method
cpg	378.56	J/mol×K	737.27	Joback Method
cpg	390.59	J/mol×K	774.89	Joback Method
cpg	402.22	J/mol×K	812.50	Joback Method
cpg	413.48	J/mol×K	850.11	Joback Method
cpg	424.42	J/mol×K	887.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435046&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume