2-Hydroxy-4,4,6-trimethylcyclohexa-2,5-dienone

Inchi: InChI=1S/C9H12O2/c1-6-4-9(2,3)5-7(10)8(6)11/h4-5,10H,1-3H3
InchiKey: GKOBUKITZSFCJC-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CC1=CC(C)(C)C=C(O)C1=O
Mol. weight [g/mol]: 152.19
CAS: 28750-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-174.89	kJ/mol	Joback Method
hf	-356.84	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	57.74	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.983		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1164.90		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1164.90		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	593.39	K	Joback Method
tc	808.90	K	Joback Method
tf	378.07	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.93	J/mol×K	593.39	Joback Method
cpg	320.94	J/mol×K	629.31	Joback Method
cpg	332.39	J/mol×K	665.23	Joback Method
cpg	343.35	J/mol×K	701.15	Joback Method
cpg	353.89	J/mol×K	737.07	Joback Method

cpg	364.09	J/mol×K	772.98	Joback Method
cpg	374.01	J/mol×K	808.90	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=C28750529&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