5-Hydroxy-2,2,6,6-tetramethyl-4-cyclohexene-1,3-d

Other names: 5-hydroxy-2,2,6,6-tetramethyl-4-cyclohexene-1,3-dione, enol form (syncarpic acid)
Inchi: InChI=1S/C10H14O3/c1-9(2)6(11)5-7(12)10(3,4)8(9)13/h5,11H,1-4H3
InchiKey: ICXMZHQQUWNXSF-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: CC1(C)C(=O)C=C(O)C(C)(C)C1=O
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
gf	-322.59	kJ/mol	Joback Method
hf	-566.59	kJ/mol	Joback Method
hfus	5.91	kJ/mol	Joback Method
hvap	61.80	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.632		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2190.00		NIST Webbook
tb	675.52	K	Joback Method
tc	904.37	K	Joback Method
tf	463.94	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.52	J/mol×K	675.52	Joback Method
cpg	417.74	J/mol×K	713.66	Joback Method
cpg	431.62	J/mol×K	751.80	Joback Method
cpg	445.32	J/mol×K	789.94	Joback Method
cpg	458.99	J/mol×K	828.09	Joback Method

cpg	472.78	J/mol×K	866.23	Joback Method
cpg	486.83	J/mol×K	904.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360321&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume