2,6-di(t-butyl)-4-hydroxy-4-methyl-2,5-cyclohexad

Other names: 2,6-di(t-Butyl)-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one
2,6-di(tert-butyl)-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one
2.6-Di(t-butyl)-4-hydroxy-4-methyl-2.5-cyclohexadien-1-one
Inchi: InChI=1S/C15H24O2/c1-13(2,3)10-8-15(7,17)9-11(12(10)16)14(4,5)6/h8-9,17H,1-7H3
InchiKey: DQBHJILNHNRDTM-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC1(O)C=C(C(C)(C)C)C(=O)C(C(C)(C)C)=C1
Mol. weight [g/mol]: 236.35
CAS: 10396-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-118.69	kJ/mol	Joback Method
hf	-498.18	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.265		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1478.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2117.00		NIST Webbook
tb	724.21	K	Joback Method
tc	941.78	K	Joback Method
tf	450.53	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.17	J/mol×K	724.21	Joback Method

cpg	638.21	J/mol×K	760.47	Joback Method
cpg	654.47	J/mol×K	796.73	Joback Method
cpg	670.09	J/mol×K	833.00	Joback Method
cpg	685.21	J/mol×K	869.26	Joback Method
cpg	699.97	J/mol×K	905.52	Joback Method
cpg	714.49	J/mol×K	941.78	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=C10396802&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
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