2,6-di-t-Butyl-4-methylene-2,5-cyclohexadiene-1-c

Inchi: InChI=1S/C15H22O/c1-10-8-11(14(2,3)4)13(16)12(9-10)15(5,6)7/h8-9H,1H2,2-7H3
InchiKey: JJQCWPWUHZFKBN-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C1C=C(C(C)(C)C)C(=O)C(C(C)(C)C)=C1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	84.41	kJ/mol	Joback Method
hf	-256.61	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.070		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	635.62	K	Joback Method
tc	864.44	K	Joback Method
tf	383.73	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.62	J/mol×K	635.62	Joback Method
cpg	554.02	J/mol×K	673.76	Joback Method
cpg	572.13	J/mol×K	711.89	Joback Method
cpg	589.01	J/mol×K	750.03	Joback Method
cpg	604.72	J/mol×K	788.17	Joback Method
cpg	619.30	J/mol×K	826.30	Joback Method
cpg	632.82	J/mol×K	864.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R278452&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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