Dl-trans-5,6-di-tert-butyl-2-hydroxy-1,4-diketo-2-cy

Inchi: InChI=1S/C14H22O3/c1-13(2,3)10-8(15)7-9(16)12(17)11(10)14(4,5)6/h7,10-11,16H,1-6H
InchiKey: PQLUOEUDBQLIIE-UHFFFAOYSA-N
Formula: C14H22O3
SMILES: CC(C)(C)C1C(=O)C=C(O)C(=O)C1C(C)(C)C
Mol. weight [g/mol]: 238.32
CAS: 3791-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-272.25	kJ/mol	Joback Method
hf	-697.13	kJ/mol	Joback Method
hfus	14.04	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.905		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
tb	760.10	K	Joback Method
tc	981.94	K	Joback Method
tf	466.06	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.88	J/mol×K	760.10	Joback Method
cpg	648.72	J/mol×K	797.07	Joback Method
cpg	664.29	J/mol×K	834.05	Joback Method
cpg	678.60	J/mol×K	871.02	Joback Method
cpg	691.67	J/mol×K	907.99	Joback Method
cpg	703.50	J/mol×K	944.97	Joback Method
cpg	714.11	J/mol×K	981.94	Joback Method

Sources

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=C3791046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume