2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol

Other names: 3,5-Bis(tert.-butyl)-4-hydroxy-propiophenon
3,5-Bis(tert.-butyl)-4-hydroxy-propiophenone
Inchi: InChI=1S/C17H26O2/c1-8-14(18)11-9-12(16(2,3)4)15(19)13(10-11)17(5,6)7/h9-10,19H,8
InchiKey: JGJQYHBWTHQSPR-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCC(=O)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 262.39
CAS: 14035-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-92.45	kJ/mol	Joback Method
hf	-488.01	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	74.20	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.580		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1644.00		NIST Webbook
ripol	2370.00		NIST Webbook
tb	753.03	K	Joback Method
tc	977.72	K	Joback Method
tf	499.30	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.92	J/mol×K	753.03	Joback Method
cpg	765.20	J/mol×K	940.27	Joback Method
cpg	751.56	J/mol×K	902.82	Joback Method

cpg	737.34	J/mol×K	865.37	Joback Method
cpg	722.42	J/mol×K	827.93	Joback Method
cpg	706.66	J/mol×K	790.48	Joback Method
cpg	778.42	J/mol×K	977.72	Joback Method
dvisc	0.0000066	Pa×s	753.03	Joback Method
dvisc	0.0000099	Pa×s	710.74	Joback Method
dvisc	0.0000156	Pa×s	668.45	Joback Method
dvisc	0.0000261	Pa×s	626.16	Joback Method
dvisc	0.0000470	Pa×s	583.88	Joback Method
dvisc	0.0000927	Pa×s	541.59	Joback Method
dvisc	0.0002052	Pa×s	499.30	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=C14035348&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
dvisc:	Dynamic viscosity
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