2,4-tert-butyl-6-hydroperoxymethyl-phenol

Inchi: InChI=1S/C15H24O3/c1-14(2,3)11-7-10(9-18-17)13(16)12(8-11)15(4,5)6/h7-8,16-17H,9H
InchiKey: KXSKHOFQSDTQAV-UHFFFAOYSA-N
Formula: C15H24O3
SMILES: CC(C)(C)c1cc(COO)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 252.35

Physical Properties

Property code	Value	Unit	Source
gf	-324.28	kJ/mol	Joback Method
hf	-684.42	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	80.17	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.977		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1744.00		NIST Webbook
tb	798.91	K	Joback Method
tc	1032.68	K	Joback Method
tf	587.43	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.42	J/mol×K	798.91	Joback Method
cpg	652.40	J/mol×K	837.87	Joback Method
cpg	665.68	J/mol×K	876.83	Joback Method
cpg	678.39	J/mol×K	915.80	Joback Method
cpg	690.71	J/mol×K	954.76	Joback Method
cpg	702.79	J/mol×K	993.72	Joback Method
cpg	714.78	J/mol×K	1032.68	Joback Method
dvisc	0.0000555	Pa×s	587.43	Joback Method
dvisc	0.0000330	Pa×s	622.68	Joback Method

dvisc	0.0000207	Pa×s	657.92	Joback Method
dvisc	0.0000136	Pa×s	693.17	Joback Method
dvisc	0.0000093	Pa×s	728.42	Joback Method
dvisc	0.0000066	Pa×s	763.66	Joback Method
dvisc	0.0000048	Pa×s	798.91	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=R169749&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume