2,4-Di-tert-butylphenol

Other names:	Phenol, 2,4-bis(1,1-dimethylethyl)-
	Phenol, 2,4-di-tert-butyl-
	2,4-di-t-Butylphenol
	1-Hydroxy-2,4-di-tert-butylbenzene
	Antioxidant No. 33
	Prodox 146
	Prodox 146A-85X
	2,4-Bis(1,1-dimethylethyl)phenol
	2,4-Bis(tert-butyl)phenol
	NSC 174502
	2,4-tert-butylphenol
	2,4-bis(1,1'-dimethylethyl)phenol
Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-7-8-12(15)11(9-10)14(4,5)6/h7-9,15H,1-6H3
InchiKey:	ICKWICRCANNIBI-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)c1ccc(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	206.32
CAS:	96-76-4

Physical Properties

Property code	Value	Unit	Source
chs	-8255.00	kJ/mol	NIST Webbook
gf	20.84	kJ/mol	Joback Method
hf	-290.00	kJ/mol	NIST Webbook
hfs	-400.00	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hsub	110.00	kJ/mol	NIST Webbook
hsub	107.10	kJ/mol	NIST Webbook
hsub	86.70 ± 0.30	kJ/mol	NIST Webbook
hsub	92.90 ± 2.80	kJ/mol	NIST Webbook
hvap	72.40 ± 0.50	kJ/mol	NIST Webbook
log10ws	-3.65		Crippen Method
logp	3.987		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1502.00		NIST Webbook

rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1511.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2318.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2316.00		NIST Webbook
tb	536.70	K	NIST Webbook
tb	538.20	K	NIST Webbook
tc	855.78	K	Joback Method
tf	403.04	K	Joback Method

vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.15	J/mol×K	625.54	Joback Method
cpg	528.92	J/mol×K	663.91	Joback Method
cpg	545.39	J/mol×K	702.29	Joback Method
cpg	560.71	J/mol×K	740.66	Joback Method
cpg	575.03	J/mol×K	779.03	Joback Method
cpg	588.49	J/mol×K	817.41	Joback Method
cpg	601.25	J/mol×K	855.78	Joback Method
dvisc	0.0004121	Pa×s	440.12	Joback Method
dvisc	0.0010791	Pa×s	403.04	Joback Method
dvisc	0.0001828	Pa×s	477.21	Joback Method
dvisc	0.0000911	Pa×s	514.29	Joback Method
dvisc	0.0000499	Pa×s	551.37	Joback Method
dvisc	0.0000295	Pa×s	588.46	Joback Method
dvisc	0.0000185	Pa×s	625.54	Joback Method
hsubt	86.10 ± 0.30	kJ/mol	307.50	NIST Webbook
hvapt	69.20 ± 0.50	kJ/mol	350.50	NIST Webbook
hvapt	60.10	kJ/mol	470.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96764&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume