2,4-Di-tert-butylphenol

Other names:	1-Hydroxy-2,4-di-tert-butylbenzene
	2,4-Bis(1,1-dimethylethyl)phenol
	2,4-Bis(tert-butyl)phenol
	2,4-bis(1,1'-dimethylethyl)phenol
	2,4-di(1,1-dimethylethyl)phenol
	2,4-di-t-Butylphenol
	2,4-tert-butylphenol
	Antioxidant No. 33
	NSC 174502
	Phenol, 2,4-bis(1,1-dimethylethyl)-
	Phenol, 2,4-di-tert-butyl-
	Prodox 146A-85X
	phenol, 2,4-di-tert-butyl
	prodox 146
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
hf	-290.00	kJ/mol	NIST Webbook
hfs	-400.00	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hsub	86.70 ± 0.30	kJ/mol	NIST Webbook
hsub	110.00	kJ/mol	NIST Webbook
hsub	107.10	kJ/mol	NIST Webbook
hsub	92.90 ± 2.80	kJ/mol	NIST Webbook
hvap	72.40 ± 0.50	kJ/mol	NIST Webbook
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-4.42		Cheméo Relay (1.0)
logp	3.987		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method

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

tc	770.78	K	Cheméo Relay (1.0)
tf	328.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-8.73100e+01
Coeff. B	1.60172e+00
Coeff. C	-1.30192e-03
Coeff. D	4.32900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc

Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.82565e+01
Coeff. B	4.60470e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	328.15
Temperature range (K), max.	599.24

Information	Value
Property code	pvap
Equation	ln(Y) = A + B/(T + C)
Y unit	kPa
Coeff. A	1.72598e+01
Coeff. B	-6.49667e+03
Coeff. C	-2.05630e+01
Reference	Stull, 1947
Comment	Coefficents calculated by NIST from author's data.
Temperature range (K), min.	357.70
Temperature range (K), max.	533.90

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

New method for determination of vaporization and sublimation enthalpy of aromatic compounds at 298.15 K using solution calorimetry technique and group-additivity scheme: https://www.doi.org/10.1016/j.tca.2015.09.022

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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

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