Phenol, 4-(1,1-dimethylethyl)-

Other names:	1-Hydroxy-4-tert-butylbenzene
	4-(1,1-dimethylethyl)phenol
	4-t-Butylphenol
	4-tert-butylphenol
	Butylphen
	NSC 3697
	PTBP
	Phenol, 4-tert-butyl-
	p-t-Butylphenol
	p-terc.Butylfenol
	p-tert-butylphenol
	phenol, p-tert-butyl-
Inchi:	InChI=1S/C10H14O/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7,11H,1-3H3
InchiKey:	QHPQWRBYOIRBIT-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	150.22
CAS:	98-54-4

Physical Properties

Property code	Value	Unit	Source
af	0.5123		Cheméo Relay (1.0)
chs	-5625.80 ± 1.20	kJ/mol	NIST Webbook
chs	-5669.00	kJ/mol	NIST Webbook
hf	-174.30	kJ/mol	NIST Webbook
hf	-214.80	kJ/mol	NIST Webbook
hf	-186.20	kJ/mol	NIST Webbook
hfs	-310.50 ± 1.20	kJ/mol	NIST Webbook
hfs	-270.00	kJ/mol	NIST Webbook
hfus	14.07	kJ/mol	Joback Method
hsub	89.40 ± 2.50	kJ/mol	NIST Webbook
hsub	95.70	kJ/mol	NIST Webbook
hsub	93.43	kJ/mol	NIST Webbook
hsub	85.90 ± 0.50	kJ/mol	NIST Webbook
hvap	67.90 ± 1.00	kJ/mol	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	8.16	eV	NIST Webbook

log10ws	-2.41		Aqueous Solubility Prediction Method
log10ws	-2.41		Estimated Solubility Method
logp	2.690		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1294.70		NIST Webbook
rinpol	1295.60		NIST Webbook
rinpol	1297.80		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1265.00		NIST Webbook
tb	503.15 ± 2.00	K	NIST Webbook
tb	510.20	K	NIST Webbook
tb	512.70	K	NIST Webbook
tb	510.65 ± 4.00	K	NIST Webbook
tb	509.65 ± 3.00	K	NIST Webbook
tb	509.00 ± 6.00	K	NIST Webbook
tb	507.65 ± 2.50	K	NIST Webbook
tb	507.65 ± 2.50	K	NIST Webbook
tb	512.88 ± 0.50	K	NIST Webbook
tb	490.65 ± 10.00	K	NIST Webbook
tb	505.15 ± 4.00	K	NIST Webbook
tc	729.89	K	Cheméo Relay (1.0)
tf	373.00 ± 1.00	K	NIST Webbook
tf	370.15 ± 3.00	K	NIST Webbook
tf	370.15 ± 3.00	K	NIST Webbook
tf	370.00 ± 3.00	K	NIST Webbook
tf	371.00 ± 3.00	K	NIST Webbook
tf	372.65 ± 2.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	373.20 ± 1.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	365.15 ± 6.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	371.40 ± 3.00	K	NIST Webbook
tf	372.90 ± 2.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook

tf	372.35 ± 1.00	K	NIST Webbook
tf	370.65 ± 3.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	371.56 ± 0.30	K	NIST Webbook
tf	372.65 ± 2.00	K	NIST Webbook
tf	372.65 ± 0.80	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	371.00 ± 5.00	K	NIST Webbook
tf	372.70 ± 3.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	373.15 ± 0.00	K	NIST Webbook
tf	372.15 ± 2.00	K	NIST Webbook
tf	371.15 ± 2.00	K	NIST Webbook
tf	371.00 ± 2.00	K	NIST Webbook
tf	372.03	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.13	J/mol×K	648.71	Joback Method
cpg	388.58	J/mol×K	765.16	Joback Method
cpg	378.53	J/mol×K	726.34	Joback Method
cpg	367.75	J/mol×K	687.53	Joback Method
cpg	314.96	J/mol×K	532.27	Joback Method
cpg	329.85	J/mol×K	571.08	Joback Method
cpg	343.53	J/mol×K	609.90	Joback Method
dvisc	0.0014227	Pa×s	374.56	Joback Method
dvisc	0.0000940	Pa×s	500.73	Joback Method
dvisc	0.0000583	Pa×s	532.27	Joback Method
dvisc	0.0038345	Pa×s	343.02	Joback Method
dvisc	0.0006157	Pa×s	406.10	Joback Method
dvisc	0.0003007	Pa×s	437.64	Joback Method
dvisc	0.0001617	Pa×s	469.19	Joback Method
hfust	14.52	kJ/mol	373.20	NIST Webbook
hfust	14.52	kJ/mol	373.20	NIST Webbook
hsubt	85.00 ± 0.50	kJ/mol	313.50	NIST Webbook

hsubt	84.30	kJ/mol	292.00	NIST Webbook
hvapt	54.30	kJ/mol	498.00	NIST Webbook
hvapt	59.60	kJ/mol	434.50	NIST Webbook
hvapt	57.60	kJ/mol	434.50	NIST Webbook
hvapt	56.60	kJ/mol	434.50	NIST Webbook
hvapt	54.40	kJ/mol	434.50	NIST Webbook
hvapt	49.90	kJ/mol	434.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54499e+01
Coeff. B	-4.64835e+03
Coeff. C	-8.37310e+01
Temperature range (K), min.	371.95
Temperature range (K), max.	542.22

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.50423e+02
Coeff. B	-1.41269e+04
Coeff. C	-1.92734e+01
Coeff. D	7.60351e-06
Temperature range (K), min.	371.56
Temperature range (K), max.	734.00

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98544&Units=SI

Chemeo Relay (1.0):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

KDB:	https://www.cheric.org/files/research/kdb/mol/mol885.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
Relationships between fusion, solution, vaporization and sublimation enthalpies of substituted phenols:	https://www.doi.org/10.1016/j.jct.2016.09.029
Solubilities of Substituted Phenols in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060058e
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=885
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point