Phenol, 4-butyl-

Other names:	1-(p-Hydroxyphenyl)butane
	1-Hydroxy-4-n-butylbenzene
	4-Butylphenol
	4-n-Butylphenol
	NSC 407848
	Phenol, p-butyl-
	p-Butylphenol
	p-Hydroxybutylbenzene
	p-n-Butylphenol
Inchi:	InChI=1S/C10H14O/c1-2-3-4-9-5-7-10(11)8-6-9/h5-8,11H,2-4H2,1H3
InchiKey:	CYYZDBDROVLTJU-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCCCc1ccc(O)cc1
Mol. weight [g/mol]:	150.22
CAS:	1638-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-8.89	kJ/mol	Joback Method
hf	-190.51	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.735		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1360.60		NIST Webbook
rinpol	1364.40		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1360.60		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1361.80		NIST Webbook
ripol	2360.00		NIST Webbook
tb	519.65 ± 3.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook

tb	512.65 ± 3.00	K	NIST Webbook
tb	516.15 ± 4.00	K	NIST Webbook
tb	513.15 ± 3.00	K	NIST Webbook
tb	518.15 ± 5.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tb	521.20	K	NIST Webbook
tb	518.15 ± 3.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tc	753.87	K	Joback Method
tf	295.15 ± 2.00	K	NIST Webbook
tf	285.15 ± 1.00	K	NIST Webbook
tf	295.15 ± 2.00	K	NIST Webbook
tf	295.15 ± 2.00	K	NIST Webbook
tf	293.65 ± 2.00	K	NIST Webbook
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/mol×K	571.90	Joback Method
cpg	338.30	J/mol×K	608.29	Joback Method
cpg	350.35	J/mol×K	644.69	Joback Method
cpg	382.17	J/mol×K	753.87	Joback Method
cpg	361.63	J/mol×K	681.08	Joback Method
cpg	372.21	J/mol×K	717.48	Joback Method
cpg	311.56	J/mol×K	535.50	Joback Method
dvisc	0.0000958	Pa×s	503.02	Joback Method
dvisc	0.0001614	Pa×s	470.53	Joback Method
dvisc	0.0002937	Pa×s	438.05	Joback Method
dvisc	0.0005881	Pa×s	405.57	Joback Method
dvisc	0.0013291	Pa×s	373.08	Joback Method
dvisc	0.0000606	Pa×s	535.50	Joback Method
dvisc	0.0035095	Pa×s	340.60	Joback Method
hvapt	49.90	kJ/mol	443.00	NIST Webbook
hvapt	54.40	kJ/mol	443.00	NIST Webbook
hvapt	57.60	kJ/mol	443.00	NIST Webbook
hvapt	61.70	kJ/mol	524.00	NIST Webbook
hvapt	56.60	kJ/mol	443.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54562e+01
Coeff. B	-4.71576e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	396.92
Temperature range (K), max.	550.88

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1638228&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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
vc:	Critical Volume