Phenol, 4-propyl-

Other names:	1-Hydroxy-4-n-propylbenzene
	4-Propylphenol
	4-n-Propylphenol
	Dihydrochavicol
	NSC 65647
	Phenol, p-propyl-
	p-Hydroxypropylbenzene
	p-Propylphenol
	p-n-Propylphenol
Inchi:	InChI=1S/C9H12O/c1-2-3-8-4-6-9(10)7-5-8/h4-7,10H,2-3H2,1H3
InchiKey:	KLSLBUSXWBJMEC-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCCc1ccc(O)cc1
Mol. weight [g/mol]:	136.19
CAS:	645-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-17.31	kJ/mol	Joback Method
hf	-169.87	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	50.92	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.345		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1259.90		NIST Webbook
rinpol	1257.50		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1231.30		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1261.70		NIST Webbook
rinpol	1231.30		NIST Webbook
rinpol	1260.40		NIST Webbook
rinpol	1235.00		NIST Webbook

rinpol	1257.50		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2250.00		NIST Webbook
tb	505.80	K	NIST Webbook
tb	504.15 ± 3.00	K	NIST Webbook
tb	505.75 ± 3.00	K	NIST Webbook
tb	505.75 ± 3.00	K	NIST Webbook
tb	506.25 ± 3.00	K	NIST Webbook
tb	507.65 ± 3.00	K	NIST Webbook
tb	502.15 ± 3.00	K	NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook
tc	734.79	K	Joback Method
tf	293.65 ± 2.00	K	NIST Webbook
tf	295.15 ± 2.00	K	NIST Webbook
tf	294.15 ± 2.00	K	NIST Webbook
tf	295.15 ± 2.00	K	NIST Webbook
tf	295.15 ± 2.00	K	NIST Webbook
tf	297.15 ± 1.00	K	NIST Webbook
tf	294.65 ± 2.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.25	J/mol×K	512.62	Joback Method
cpg	280.20	J/mol×K	549.65	Joback Method
cpg	292.23	J/mol×K	586.68	Joback Method
cpg	303.43	J/mol×K	623.70	Joback Method
cpg	313.87	J/mol×K	660.73	Joback Method
cpg	323.62	J/mol×K	697.76	Joback Method
cpg	332.77	J/mol×K	734.79	Joback Method
dvisc	0.0000766	Pa×s	512.62	Joback Method
dvisc	0.0016445	Pa×s	359.88	Joback Method
dvisc	0.0007350	Pa×s	390.43	Joback Method
dvisc	0.0042723	Pa×s	329.33	Joback Method
dvisc	0.0002036	Pa×s	451.52	Joback Method
dvisc	0.0001211	Pa×s	482.07	Joback Method

dvisc	0.0003692	Pa×s	420.98	Joback Method
hvapt	56.70	kJ/mol	445.50	NIST Webbook
hvapt	61.30	kJ/mol	432.00	NIST Webbook
hvapt	59.50	kJ/mol	432.00	NIST Webbook
hvapt	58.40	kJ/mol	432.00	NIST Webbook
hvapt	56.20	kJ/mol	432.00	NIST Webbook
hvapt	51.50	kJ/mol	432.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55943e+01
Coeff. B	-4.64285e+03
Coeff. C	-8.19990e+01
Temperature range (K), min.	385.32
Temperature range (K), max.	533.51

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645567&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
Effect of Isomers on Partition Coefficients for Phenolic Compounds in the 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water Two-Phase System:	https://www.doi.org/10.1021/je100016z
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume