Phenol, 4-pentyl-

Other names:	4-Amylphenol
	4-Pentylphenol
	4-n-Amylphenol
	4-n-Pentylphenol
	Amyl p-hydroxybenzene
	Phenol, p-pentyl-
	p-Amylphenol
	p-Hydroxy-n-pentylbenzene
	p-Pentylphenol
	p-n-Amylphenol
Inchi:	InChI=1S/C11H16O/c1-2-3-4-5-10-6-8-11(12)9-7-10/h6-9,12H,2-5H2,1H3
InchiKey:	ZNPSUQQXTRRSBM-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCCCCc1ccc(O)cc1
Mol. weight [g/mol]:	164.24
CAS:	14938-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-0.47	kJ/mol	Joback Method
hf	-211.15	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	55.37	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.125		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1462.50		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1465.90		NIST Webbook
ripol	2461.00		NIST Webbook
ripol	2461.00		NIST Webbook
tb	558.38	K	Joback Method
tc	773.05	K	Joback Method
tf	291.15 ± 1.00	K	NIST Webbook
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.61	J/mol×K	558.38	Joback Method
cpg	372.22	J/mol×K	594.16	Joback Method
cpg	385.88	J/mol×K	629.94	Joback Method
cpg	398.69	J/mol×K	665.71	Joback Method
cpg	410.71	J/mol×K	701.49	Joback Method
cpg	422.03	J/mol×K	737.27	Joback Method
cpg	432.71	J/mol×K	773.05	Joback Method
dvisc	0.0028753	Pa×s	351.87	Joback Method
dvisc	0.0010731	Pa×s	386.29	Joback Method
dvisc	0.0004706	Pa×s	420.71	Joback Method
dvisc	0.0002338	Pa×s	455.12	Joback Method
dvisc	0.0001281	Pa×s	489.54	Joback Method
dvisc	0.0000760	Pa×s	523.96	Joback Method
dvisc	0.0000481	Pa×s	558.38	Joback Method
hvapt	60.90	kJ/mol	493.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56026e+01
Coeff. B	-4.78128e+03
Coeff. C	-8.67250e+01
Temperature range (K), min.	398.92
Temperature range (K), max.	551.33

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14938353&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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