Phenol, 4-hexyl-

Other names:	p-Hexylphenol
	p-n-Hexylphenol
	4-n-Hexylphenol
	4-Hexylphenol
Inchi:	InChI=1S/C12H18O/c1-2-3-4-5-6-11-7-9-12(13)10-8-11/h7-10,13H,2-6H2,1H3
InchiKey:	SZWBRVPZWJYIHI-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCCCCCc1ccc(O)cc1
Mol. weight [g/mol]:	178.27
CAS:	2446-69-7

Physical Properties

Property code	Value	Unit	Source
gf	7.95	kJ/mol	Joback Method
hf	-231.79	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	57.60	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.515		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1568.80		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1561.60		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1561.60		NIST Webbook
tb	581.26	K	Joback Method
tc	792.37	K	Joback Method
tf	302.15 ± 1.00	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.33	J/mol×K	581.26	Joback Method
cpg	473.05	J/mol×K	757.18	Joback Method
cpg	461.08	J/mol×K	722.00	Joback Method
cpg	448.40	J/mol×K	686.81	Joback Method
cpg	434.94	J/mol×K	651.63	Joback Method
cpg	420.60	J/mol×K	616.44	Joback Method
cpg	484.37	J/mol×K	792.37	Joback Method
dvisc	0.0000382	Pa×s	581.26	Joback Method
dvisc	0.0000604	Pa×s	544.91	Joback Method
dvisc	0.0001019	Pa×s	508.55	Joback Method
dvisc	0.0001863	Pa×s	472.20	Joback Method
dvisc	0.0003767	Pa×s	435.85	Joback Method
dvisc	0.0008660	Pa×s	399.49	Joback Method
dvisc	0.0023516	Pa×s	363.14	Joback Method

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=C2446697&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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