Phenol, 4-heptyl-

Other names:	4-heptylphenol
	4-n-Heptylphenol
	p-Heptylphenol
	p-n-Heptylphenol
Inchi:	InChI=1S/C13H20O/c1-2-3-4-5-6-7-12-8-10-13(14)11-9-12/h8-11,14H,2-7H2,1H3
InchiKey:	KNDDEFBFJLKPFE-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	CCCCCCCc1ccc(O)cc1
Mol. weight [g/mol]:	192.30
CAS:	1987-50-4

Physical Properties

Property code	Value	Unit	Source
gf	16.37	kJ/mol	Joback Method
hf	-252.43	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	59.82	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.905		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1665.50		NIST Webbook
rinpol	1665.50		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1673.80		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2679.00		NIST Webbook
tb	604.14	K	Joback Method
tc	811.88	K	Joback Method
tf	297.15 ± 2.00	K	NIST Webbook
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.63	J/mol×K	604.14	Joback Method
cpg	525.24	J/mol×K	777.26	Joback Method
cpg	512.69	J/mol×K	742.64	Joback Method
cpg	499.44	J/mol×K	708.01	Joback Method
cpg	485.39	J/mol×K	673.39	Joback Method
cpg	470.48	J/mol×K	638.76	Joback Method
cpg	537.14	J/mol×K	811.88	Joback Method
dvisc	0.0000305	Pa×s	604.14	Joback Method
dvisc	0.0000481	Pa×s	565.85	Joback Method
dvisc	0.0000812	Pa×s	527.56	Joback Method
dvisc	0.0001487	Pa×s	489.27	Joback Method
dvisc	0.0003019	Pa×s	450.99	Joback Method
dvisc	0.0006989	Pa×s	412.70	Joback Method
dvisc	0.0019211	Pa×s	374.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47195e+01
Coeff. B	-4.59108e+03
Coeff. C	-8.98800e+01
Temperature range (K), min.	408.00
Temperature range (K), max.	577.88

Sources

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=C1987504&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

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
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