Phenol, 3-pentadecyl-

Other names:	3-n-Pentadecylphenol
	3-pentadecylphenol
	Anacardol, tetrahydro-
	Cardolite NC-507
	Cardolite NC-510
	Cyclogallipharaol
	Hydroginkgol
	NSC 9781
	hydrocardanol
	m-pentadecylphenol
	phenol, m-pentadecyl-
	tetrahydroanacardol
Inchi:	InChI=1S/C21H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-20-17-15-18-21(22)19-20/h15
InchiKey:	PTFIPECGHSYQNR-UHFFFAOYSA-N
Formula:	C21H36O
SMILES:	CCCCCCCCCCCCCCCc1cccc(O)c1
Mol. weight [g/mol]:	304.51
CAS:	501-24-6

Physical Properties

Property code	Value	Unit	Source
gf	83.73	kJ/mol	Joback Method
hf	-417.55	kJ/mol	Joback Method
hfus	38.09	kJ/mol	Solubilities of 3-Pentadecylphenol in Ethanol, 1-Butanol, Toluene, Acetone, Tetrachloromethane, and Ethyl Acetate
hvap	77.63	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	7.026		Crippen Method
mcvol	288.860	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2499.80		NIST Webbook
rinpol	2499.80		NIST Webbook
tb	787.18	K	Joback Method
tc	980.56	K	Joback Method

tf	325.20 ± 1.50	K	NIST Webbook
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.46	J/mol×K	787.18	Joback Method
cpg	915.30	J/mol×K	819.41	Joback Method
cpg	933.25	J/mol×K	851.64	Joback Method
cpg	950.39	J/mol×K	883.87	Joback Method
cpg	966.79	J/mol×K	916.10	Joback Method
cpg	982.54	J/mol×K	948.33	Joback Method
cpg	997.72	J/mol×K	980.56	Joback Method
dvisc	0.0003779	Pa×s	464.57	Joback Method
dvisc	0.0001284	Pa×s	518.34	Joback Method
dvisc	0.0000534	Pa×s	572.11	Joback Method
dvisc	0.0000259	Pa×s	625.88	Joback Method
dvisc	0.0000140	Pa×s	679.64	Joback Method
dvisc	0.0000083	Pa×s	733.41	Joback Method
dvisc	0.0000053	Pa×s	787.18	Joback Method
hfust	38.09	kJ/mol	322.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.70	K	0.10	NIST Webbook
tbrp	470.20	K	0.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C501246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of 3-Pentadecylphenol in Ethanol, 1-Butanol, Toluene, Acetone, Tetrachloromethane, and Ethyl Acetate:	https://www.doi.org/10.1021/je900346t

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
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume