

Phenol, 4-dodecyl-

Other names:	4-Dodecylphenol Phenol, p-dodecyl- p-Dodecylphenol
Inchi:	InChI=1S/C18H30O/c1-2-3-4-5-6-7-8-9-10-11-12-17-13-15-18(19)16-14-17/h13-16,19H,2
InchiKey:	KJWMCPYEODZESQ-UHFFFAOYSA-N
Formula:	C18H30O
SMILES:	CCCCCCCCCCCCc1ccc(O)cc1
Mol. weight [g/mol]:	262.43
CAS:	104-43-8

Physical Properties

Property code	Value	Unit	Source
gf	58.47	kJ/mol	Joback Method
hf	-355.63	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	70.95	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.856		Crippen Method
mcvol	246.590	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	718.54	K	Joback Method
tc	914.00	K	Joback Method
tf	430.76	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.95	J/molxK	718.54	Joback Method
cpg	802.98	J/molxK	881.43	Joback Method
cpg	788.29	J/molxK	848.85	Joback Method
cpg	772.92	J/molxK	816.27	Joback Method

cpg	756.79	J/molxK	783.69	Joback Method
cpg	739.82	J/molxK	751.12	Joback Method
cpg	817.06	J/molxK	914.00	Joback Method
dvisc	0.0000101	Paxs	718.54	Joback Method
dvisc	0.0000159	Paxs	670.58	Joback Method
dvisc	0.0000268	Paxs	622.61	Joback Method
dvisc	0.0000493	Paxs	574.65	Joback Method
dvisc	0.0001014	Paxs	526.69	Joback Method
dvisc	0.0002411	Paxs	478.72	Joback Method
dvisc	0.0006949	Paxs	430.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41722e+01
Coeff. B	-4.69348e+03
Coeff. C	-1.00486e+02
Temperature range (K), min.	438.15
Temperature range (K), max.	630.15

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=C104438&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/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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