P-DODECYLPHENOL

Other names: 4-Dodecylphenol
Phenol, p-dodecyl-
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]: 262.44
CAS: 104-43-8

Physical Properties

Property code	Value	Unit	Source
af	0.9174		Cheméo Relay (1.0)
gf	58.47	kJ/mol	Joback Method
hf	-339.82	kJ/mol	Cheméo Relay (1.0)
hfus	42.20	kJ/mol	Joback Method
hvap	107.33	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-6.23		Cheméo Relay (1.0)
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	620.43	K	Cheméo Relay (1.0)
tc	822.11	K	Cheméo Relay (1.0)
tf	336.14	K	Cheméo Relay (1.0)
vc	0.929	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.95	J/mol×K	718.54	Joback Method
cpg	739.82	J/mol×K	751.12	Joback Method
cpg	756.79	J/mol×K	783.69	Joback Method

cpg	772.92	J/mol×K	816.27	Joback Method
cpg	788.29	J/mol×K	848.85	Joback Method
cpg	802.98	J/mol×K	881.43	Joback Method
cpg	817.06	J/mol×K	914.00	Joback Method
dvisc	0.0006949	Pa×s	430.76	Joback Method
dvisc	0.0002411	Pa×s	478.72	Joback Method
dvisc	0.0001014	Pa×s	526.69	Joback Method
dvisc	0.0000493	Pa×s	574.65	Joback Method
dvisc	0.0000268	Pa×s	622.61	Joback Method
dvisc	0.0000159	Pa×s	670.58	Joback Method
dvisc	0.0000101	Pa×s	718.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104438&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume