2-n-HEXYLPHENOL

Other names:	2-Hexylphenol
	Phenol, 2-hexyl-
	Phenol, o-hexyl-
	o-Hexylphenol
Inchi:	InChI=1S/C12H18O/c1-2-3-4-5-8-11-9-6-7-10-12(11)13/h6-7,9-10,13H,2-5,8H2,1H3
InchiKey:	ABMULKFGWTYIIK-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCCCCCc1ccccc1O
Mol. weight [g/mol]:	178.28
CAS:	3226-32-2

Physical Properties

Property code	Value	Unit	Source
af	0.6696		Cheméo Relay (1.0)
gf	7.95	kJ/mol	Joback Method
hf	-218.94	kJ/mol	Cheméo Relay (1.0)
hfus	26.66	kJ/mol	Joback Method
hvap	75.79	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	3.515		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	538.26	K	Cheméo Relay (1.0)
tc	754.27	K	Cheméo Relay (1.0)
tf	292.12	K	Cheméo Relay (1.0)
vc	0.590	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.33	J/mol×K	581.26	Joback Method
cpg	420.60	J/mol×K	616.44	Joback Method
cpg	434.94	J/mol×K	651.63	Joback Method

cpg	448.40	J/mol×K	686.81	Joback Method
cpg	461.08	J/mol×K	722.00	Joback Method
cpg	473.05	J/mol×K	757.18	Joback Method
cpg	484.37	J/mol×K	792.37	Joback Method
dvisc	0.0023516	Pa×s	363.14	Joback Method
dvisc	0.0008660	Pa×s	399.49	Joback Method
dvisc	0.0003767	Pa×s	435.85	Joback Method
dvisc	0.0001863	Pa×s	472.20	Joback Method
dvisc	0.0001019	Pa×s	508.55	Joback Method
dvisc	0.0000604	Pa×s	544.91	Joback Method
dvisc	0.0000382	Pa×s	581.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47121e+01
Coeff. B	-4.50797e+03
Coeff. C	-8.68980e+01
Temperature range (K), min.	399.42
Temperature range (K), max.	566.44

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3226322&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):	

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