

Nonylphenol

Other names:	Phenol, nonyl-
Inchi:	InChI=1S/C15H24O/c1-11(2)9-12(3)10-13(4)14-5-7-15(16)8-6-14/h5-8,11-13,16H,9-10H2
InchiKey:	SLULBVLEUPOSOI-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC(C)CC(C)CC(C)c1ccc(O)cc1
Mol. weight [g/mol]:	220.35
CAS:	25154-52-3

Physical Properties

Property code	Value	Unit	Source
gf	25.89	kJ/mol	Joback Method
hf	-309.55	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	2155.30	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	648.58	K	Joback Method
tc	861.97	K	Joback Method
tf	351.95	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.96	J/molxK	648.58	Joback Method
cpg	576.84	J/molxK	684.14	Joback Method
cpg	593.65	J/molxK	719.71	Joback Method
cpg	609.47	J/molxK	755.27	Joback Method

cpg	624.40	J/molxK	790.84	Joback Method
cpg	638.52	J/molxK	826.40	Joback Method
cpg	651.91	J/molxK	861.97	Joback Method
dvisc	0.0046742	Paxs	351.95	Joback Method
dvisc	0.0010084	Paxs	401.39	Joback Method
dvisc	0.0003045	Paxs	450.83	Joback Method
dvisc	0.0001165	Paxs	500.26	Joback Method
dvisc	0.0000530	Paxs	549.70	Joback Method
dvisc	0.0000275	Paxs	599.14	Joback Method
dvisc	0.0000157	Paxs	648.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.80470e+01
Coeff. B	-6.16655e+03
Coeff. C	-1.05381e+02
Temperature range (K), min.	452.61
Temperature range (K), max.	589.58

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.35332e+02
Coeff. B	-1.58023e+04
Coeff. C	-1.65004e+01
Coeff. D	4.43190e-06
Temperature range (K), min.	279.15
Temperature range (K), max.	757.00

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Joback Method:

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

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=891
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25154523&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=891

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
nfpa:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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