Phenol, 2,6-dimethyl-

Other names:	1,2,6-Xylenol
	1,3-Dimethyl-2-hydroxybenzene
	1-HYDROXY-2,6-DIMETHYLBENZENE
	2,6-DIMETHYLPHENOL
	2,6-Dmp
	2,6-Xylenol
	NSC 2123
Inchi:	InChI=1S/C8H10O/c1-6-4-3-5-7(2)8(6)9/h3-5,9H,1-2H3
InchiKey:	NXXYKOUNUYWIHA-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1cccc(C)c1O
Mol. weight [g/mol]:	122.16
CAS:	576-26-1

Physical Properties

Property code	Value	Unit	Source
chs	-4344.20 ± 2.90	kJ/mol	NIST Webbook
chs	-4339.90 ± 1.00	kJ/mol	NIST Webbook
chs	-4325.40	kJ/mol	NIST Webbook
gf	-35.36	kJ/mol	Joback Method
hf	-161.80 ± 0.54	kJ/mol	NIST Webbook
hf	-174.40	kJ/mol	NIST Webbook
hf	-157.50	kJ/mol	NIST Webbook
hf	-161.90	kJ/mol	KDB
hfs	-237.40 ± 1.10	kJ/mol	NIST Webbook
hfs	-233.10 ± 2.90	kJ/mol	NIST Webbook
hfs	-250.00	kJ/mol	NIST Webbook
hfus	15.91	kJ/mol	Joback Method
hsub	59.40 ± 0.80	kJ/mol	NIST Webbook
hsub	75.60	kJ/mol	NIST Webbook
hsub	75.10	kJ/mol	NIST Webbook
hsub	75.60	kJ/mol	NIST Webbook
hsub	75.60 ± 0.20	kJ/mol	NIST Webbook
hvap	75.60	kJ/mol	NIST Webbook
hvap	75.31	kJ/mol	NIST Webbook
hvap	75.10	kJ/mol	NIST Webbook
ie	8.34	eV	NIST Webbook

ie	8.05 ± 0.02	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
log10ws	-1.31		Aqueous Solubility Prediction Method
log10ws	-1.29		Estimated Solubility Method
logp	2.009		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
rinpol	1105.50		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1115.77		NIST Webbook
rinpol	1080.49		NIST Webbook
rinpol	1081.07		NIST Webbook
rinpol	1081.55		NIST Webbook
rinpol	1082.02		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1083.07		NIST Webbook
rinpol	1087.90		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1084.10		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1102.30		NIST Webbook
rinpol	1104.60		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1080.50		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1102.30		NIST Webbook
rinpol	1104.60		NIST Webbook
rinpol	1105.50		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1082.12		NIST Webbook
rinpol	1077.41		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.41		NIST Webbook
rinpol	1130.00		NIST Webbook

rinpol	1117.00		NIST Webbook
rinpol	1114.20		NIST Webbook
rinpol	1114.90		NIST Webbook
rinpol	1117.20		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1106.31		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	184.51		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	184.51		NIST Webbook
rinpol	182.30		NIST Webbook
rinpol	184.08		NIST Webbook
rinpol	184.08		NIST Webbook
rinpol	1108.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1918.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1917.00		NIST Webbook
tb	474.22	K	KDB
tc	701.00	K	KDB
tc	700.95 ± 0.20	K	NIST Webbook
tf	320.57	K	Aqueous Solubility Prediction Method
tf	318.80	K	KDB
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.69	J/mol×K	684.14	Joback Method
cpg	282.81	J/mol×K	722.03	Joback Method
cpg	224.69	J/mol×K	494.72	Joback Method
cpg	236.18	J/mol×K	532.60	Joback Method
cpg	246.85	J/mol×K	570.49	Joback Method
cpg	256.78	J/mol×K	608.37	Joback Method
cpg	266.04	J/mol×K	646.26	Joback Method
dvisc	0.0001358	Pa×s	467.36	Joback Method
dvisc	0.0000891	Pa×s	494.72	Joback Method
dvisc	0.0031710	Pa×s	330.58	Joback Method
dvisc	0.0013928	Pa×s	357.94	Joback Method
dvisc	0.0006876	Pa×s	385.29	Joback Method
dvisc	0.0003727	Pa×s	412.65	Joback Method
dvisc	0.0002180	Pa×s	440.01	Joback Method
hfust	18.90	kJ/mol	318.90	NIST Webbook
hfust	18.90	kJ/mol	318.90	NIST Webbook
hfust	18.90	kJ/mol	318.90	NIST Webbook
hfust	18.83	kJ/mol	318.60	NIST Webbook
hsubt	75.60 ± 0.17	kJ/mol	295.00	NIST Webbook
hvapt	48.50	kJ/mol	446.50	NIST Webbook
sfust	59.26	J/mol×K	318.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	390.06	K	6.70	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa

tbp	396.14	K	8.87	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	401.43	K	10.89	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	405.64	K	12.74	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	409.97	K	14.98	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	413.33	K	16.80	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	416.65	K	18.91	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	

tbp	419.43	K	21.02	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	422.01	K	22.83	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	436.55	K	33.02	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	438.90	K	35.64	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	
tbp	418.11	K	20.00	Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.54388e+01
Coeff. B	-4.33921e+03
Coeff. C	-7.29830e+01
Temperature range (K), min.	359.38
Temperature range (K), max.	501.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.30489e+02
Coeff. B	-1.16579e+04
Coeff. C	-1.67611e+01
Coeff. D	8.86220e-06
Temperature range (K), min.	318.76
Temperature range (K), max.	701.05

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and correlation of isobaric vapour-liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa:	https://www.doi.org/10.1016/j.fluid.2017.12.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=877
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C576261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol877.mol
Thermochemistry of Li, Na, K, Rb and Cs alkylated phenoxides:	https://www.doi.org/10.1016/j.tca.2005.02.027

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume