Phenol, 2,4-dimethyl-

Other names:	1,3-Dimethyl-4-hydroxybenzene
	1-HYDROXY-2,4-DIMETHYLBENZENE
	2,4-DIMETHYLPHENOL
	2,4-Xylenol
	4,6-Dimethylphenol
	4-Hydroxy-1,3-dimethylbenzene
	NSC 3829
	Rcra waste number U101
	m-Xylenol
Inchi:	InChI=1S/C8H10O/c1-6-3-4-8(9)7(2)5-6/h3-5,9H,1-2H3
InchiKey:	KUFFULVDNCHOFZ-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1ccc(O)c(C)c1
Mol. weight [g/mol]:	122.16
CAS:	105-67-9

Physical Properties

Property code	Value	Unit	Source
chl	-4348.47 ± 0.92	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
gf	-35.36	kJ/mol	Joback Method
hf	-163.00 ± 0.75	kJ/mol	NIST Webbook
hf	-162.80	kJ/mol	KDB
hfl	-228.80 ± 1.40	kJ/mol	NIST Webbook
hfus	15.91	kJ/mol	Joback Method
hvap	48.53	kJ/mol	NIST Webbook
hvap	65.80	kJ/mol	NIST Webbook
hvap	65.90 ± 0.20	kJ/mol	NIST Webbook
hvap	64.60	kJ/mol	NIST Webbook
hvap	64.96	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
log10ws	-1.19		Estimated Solubility Method
log10ws	-1.19		Aqueous Solubility Prediction Method
logp	2.009		Crippen Method

mcvol	105.690	ml/mol	McGowan Method
pc	10132.50 ± 0.50	kPa	NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1148.90		NIST Webbook
rinpol	1150.10		NIST Webbook
rinpol	1151.40		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	192.69		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook

rinpol	1134.00		NIST Webbook
rinpol	192.24		NIST Webbook
rinpol	190.90		NIST Webbook
rinpol	191.20		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1181.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2098.97		NIST Webbook
ripol	2098.02		NIST Webbook
ripol	2094.74		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2098.99		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2078.00		NIST Webbook
tb	484.13	K	KDB
tc	707.60	K	KDB
tc	707.55 ± 0.30	K	NIST Webbook
tc	818.15 ± 2.00	K	NIST Webbook
tf	297.68	K	KDB
tf	297.65	K	Aqueous Solubility Prediction Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.69	J/mol×K	494.72	Joback Method
cpg	246.85	J/mol×K	570.49	Joback Method
cpg	282.81	J/mol×K	722.03	Joback Method
cpg	256.78	J/mol×K	608.37	Joback Method
cpg	266.04	J/mol×K	646.26	Joback Method
cpg	274.69	J/mol×K	684.14	Joback Method
cpg	236.18	J/mol×K	532.60	Joback Method
dvisc	0.0001358	Pa×s	467.36	Joback Method
dvisc	0.0002180	Pa×s	440.01	Joback Method
dvisc	0.0003727	Pa×s	412.65	Joback Method
dvisc	0.0006876	Pa×s	385.29	Joback Method

dvisc	0.0013928	Pa×s	357.94	Joback Method
dvisc	0.0000891	Pa×s	494.72	Joback Method
dvisc	0.0031710	Pa×s	330.58	Joback Method
hfust	12.76	kJ/mol	297.30	NIST Webbook
hsubt	61.50 ± 0.80	kJ/mol	310.00	NIST Webbook
hvapt	65.90 ± 0.20	kJ/mol	300.00	NIST Webbook
hvapt	65.90 ± 0.20	kJ/mol	300.00	NIST Webbook
hvapt	65.90	kJ/mol	300.00	NIST Webbook
hvapt	51.80	kJ/mol	457.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54387e+01
Coeff. B	-4.41754e+03
Coeff. C	-7.57380e+01
Temperature range (K), min.	367.30
Temperature range (K), max.	511.94

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.35548e+02
Coeff. B	-1.25596e+04
Coeff. C	-1.72828e+01
Coeff. D	7.98314e-06
Temperature range (K), min.	345.71
Temperature range (K), max.	707.65

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=875
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid Equilibrium Measurements for Model Systems Related to Catalytic Fast Pyrolysis of Biomass:	https://www.doi.org/10.1021/acs.jced.6b00625
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105679&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=875
KDB:	https://www.cheric.org/files/research/kdb/mol/mol875.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume