Phenol, 2,3-dimethyl-

Other names:	1,2-Dimethyl-3-hydroxybenzene
	1-HYDROXY-2,3-DIMETHYLBENZENE
	2,3-DIMETHYLPHENOL
	2,3-Xylenol
	NSC 62011
	o-Xylenol
Inchi:	InChI=1S/C8H10O/c1-6-4-3-5-8(9)7(6)2/h3-5,9H,1-2H3
InchiKey:	QWBBPBRQALCEIZ-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1cccc(O)c1C
Mol. weight [g/mol]:	122.16
CAS:	526-75-0

Physical Properties

Property code	Value	Unit	Source
chs	-4336.00 ± 0.92	kJ/mol	NIST Webbook
gf	-35.36	kJ/mol	Joback Method
hf	-157.30 ± 1.10	kJ/mol	NIST Webbook
hf	-157.30	kJ/mol	KDB
hfs	-241.30 ± 1.10	kJ/mol	NIST Webbook
hfus	15.91	kJ/mol	Joback Method
hsub	84.00 ± 1.00	kJ/mol	NIST Webbook
hsub	84.00	kJ/mol	NIST Webbook
hsub	59.40 ± 0.80	kJ/mol	NIST Webbook
hvap	49.35	kJ/mol	Joback Method
ie	8.26	eV	NIST Webbook
log10ws	-1.43		Aqueous Solubility Prediction Method
logp	2.009		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	198.95		NIST Webbook
rinpol	198.65		NIST Webbook
rinpol	198.95		NIST Webbook
rinpol	1167.00		NIST Webbook

rinpol	1169.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	196.80		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1190.60		NIST Webbook
rinpol	1178.90		NIST Webbook
rinpol	1180.10		NIST Webbook
rinpol	1182.20		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	198.03		NIST Webbook
ripol	2147.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2140.00		NIST Webbook
ripol	2147.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2147.00		NIST Webbook
tb	491.15 ± 2.00	K	NIST Webbook
tb	490.07	K	KDB
tb	491.20 ± 2.00	K	NIST Webbook

tb	491.15 ± 2.00	K	NIST Webbook
tb	490.95 ± 2.00	K	NIST Webbook
tb	491.15 ± 3.00	K	NIST Webbook
tb	490.25 ± 2.00	K	NIST Webbook
tb	492.15 ± 3.00	K	NIST Webbook
tb	491.20	K	NIST Webbook
tb	484.65 ± 5.00	K	NIST Webbook
tc	722.85 ± 0.40	K	NIST Webbook
tc	722.80	K	KDB
tf	345.91	K	Aqueous Solubility Prediction Method
tf	345.90	K	KDB
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	274.69	J/mol×K	684.14	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
dvisc	0.0001358	Pa×s	467.36	Joback Method
hfust	21.02	kJ/mol	346.00	NIST Webbook
hfust	21.02	kJ/mol	346.00	NIST Webbook
hfust	20.29	kJ/mol	345.80	NIST Webbook
hfust	21.02	kJ/mol	346.00	NIST Webbook
hsubt	61.50 ± 0.80	kJ/mol	310.00	NIST Webbook
hsubt	84.00 ± 1.00	kJ/mol	303.00	NIST Webbook
hvapt	52.10	kJ/mol	462.50	NIST Webbook
sfust	60.76	J/mol×K	346.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54381e+01
Coeff. B	-4.46433e+03
Coeff. C	-7.73890e+01
Temperature range (K), min.	345.71
Temperature range (K), max.	518.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05582e+02
Coeff. B	-1.07419e+04
Coeff. C	-1.30204e+01
Coeff. D	6.74763e-06
Temperature range (K), min.	345.71
Temperature range (K), max.	722.95

Sources

Solubilities of Substituted Phenols in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060058e
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=874
Experiments and COSMO-SAC Modeling of Methyl Isobutyl Ketone + Dimethylphenols + Water Mixtures:	https://www.doi.org/10.1021/acs.jced.9b00300
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Formation of Deep Eutectic Solvents by Phenols and Choline Chloride and Their Physical Properties:	https://www.doi.org/10.1021/je300997v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol874.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C526750&Units=SI

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