Phenol, 2,5-dimethyl-

Other names:	1,2,5-Xylenol
	1,4-Dimethyl-2-hydroxybenzene
	1-HYDROXY-2,5-DIMETHYLBENZENE
	2,5-DIMETHYLPHENOL
	2,5-Dmp
	2,5-Xylenol
	2-Hydroxy-p-xylene
	3,6-Dimethylphenol
	3,6-Xylenol
	6-Methyl-m-cresol
	NSC 2599
	p-Xylenol
Inchi:	InChI=1S/C8H10O/c1-6-3-4-7(2)8(9)5-6/h3-5,9H,1-2H3
InchiKey:	NKTOLZVEWDHZMU-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1ccc(C)c(O)c1
Mol. weight [g/mol]:	122.16
CAS:	95-87-4

Physical Properties

Property code	Value	Unit	Source
chs	-4330.61 ± 0.92	kJ/mol	NIST Webbook
dm	1.50	debye	KDB
gf	-35.36	kJ/mol	Joback Method
hf	-161.50	kJ/mol	KDB
hf	-161.70 ± 0.50	kJ/mol	NIST Webbook
hfs	-246.30 ± 1.00	kJ/mol	NIST Webbook
hfus	15.91	kJ/mol	Joback Method
hsub	85.00 ± 0.30	kJ/mol	NIST Webbook
hsub	84.60	kJ/mol	NIST Webbook
hvap	49.35	kJ/mol	Joback Method
log10ws	-1.54		Aqueous Solubility Prediction Method
logp	2.009		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
rinpol	1125.00		NIST Webbook

rinpol	1150.90		NIST Webbook
rinpol	1151.80		NIST Webbook
rinpol	1153.50		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1124.80		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	192.82		NIST Webbook
rinpol	190.90		NIST Webbook
rinpol	192.94		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2066.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2085.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2086.00		NIST Webbook
tb	484.33	K	KDB
tc	706.90 ± 0.20	K	NIST Webbook
tc	723.05 ± 0.50	K	NIST Webbook
tc	706.90	K	KDB

tf	347.90	K	KDB
tf	348.27	K	Aqueous Solubility Prediction Method
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	256.78	J/mol×K	608.37	Joback Method
cpg	246.85	J/mol×K	570.49	Joback Method
cpg	236.18	J/mol×K	532.60	Joback Method
cpg	224.69	J/mol×K	494.72	Joback Method
cpg	282.81	J/mol×K	722.03	Joback Method
cpg	266.04	J/mol×K	646.26	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
dvisc	0.0031710	Pa×s	330.58	Joback Method
dvisc	0.0000891	Pa×s	494.72	Joback Method
hfust	13.81	kJ/mol	348.10	NIST Webbook
hfust	23.38	kJ/mol	348.00	NIST Webbook
hfust	23.38	kJ/mol	348.00	NIST Webbook
hfust	23.38	kJ/mol	348.00	NIST Webbook
hsubt	64.00 ± 0.80	kJ/mol	348.00	NIST Webbook
hsubt	85.00 ± 0.25	kJ/mol	302.50	NIST Webbook
hvapt	51.70	kJ/mol	456.00	NIST Webbook
sfust	67.17	J/mol×K	348.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54574e+01
Coeff. B	-4.42459e+03

Coeff. C	-7.57940e+01
Temperature range (K), min.	347.99
Temperature range (K), max.	511.89

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.27627e+02
Coeff. B	-1.20343e+04
Coeff. C	-1.61842e+01
Coeff. D	8.17909e-06
Temperature range (K), min.	347.99
Temperature range (K), max.	707.05

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95874&Units=SI

Solubilities of Substituted Phenols in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je060058e

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=876

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB: https://www.cheric.org/files/research/kdb/mol/mol876.mol

Legend

chs: Standard solid 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

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
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