PHENOL, 3,4-DIMETHYL-

Other names:	1,2-Dimethyl-4-hydroxybenzene
	1,3,4-Xylenol
	1-hydroxy-3,4-dimethylbenzene
	3,4-DMP
	3,4-dimethylphenol
	3,4-xylenol
	4,5-Dimethylphenol
	4-Hydroxy-1,2-dimethylbenzene
	NSC 1549
Inchi:	InChI=1S/C8H10O/c1-6-3-4-8(9)5-7(6)2/h3-5,9H,1-2H3
InchiKey:	YCOXTKKNXUZSKD-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1ccc(O)cc1C
Mol. weight [g/mol]:	122.17
CAS:	95-65-8

Physical Properties

Property code	Value	Unit	Source
af	0.5214		Cheméo Relay (1.0)
chs	-4334.90 ± 1.10	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	-35.36	kJ/mol	Joback Method
hf	-156.60 ± 0.59	kJ/mol	NIST Webbook
hf	-156.50	kJ/mol	KDB
hfs	-242.40 ± 0.59	kJ/mol	NIST Webbook
hfus	15.91	kJ/mol	Joback Method
hsub	85.70 ± 0.10	kJ/mol	NIST Webbook
hsub	85.00	kJ/mol	NIST Webbook
hsub	85.80	kJ/mol	NIST Webbook
hsub	85.00	kJ/mol	NIST Webbook
hsub	85.10	kJ/mol	NIST Webbook
hvap	45.61	kJ/mol	NIST Webbook
hvap	85.03	kJ/mol	NIST Webbook
hvap	85.00	kJ/mol	NIST Webbook
hvap	85.10	kJ/mol	NIST Webbook
ie	8.09	eV	NIST Webbook

log10ws	-1.41		Aqueous Solubility Prediction Method
log10ws	-1.38		Estimated Solubility Method
logp	2.009		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	6586.12 ± 303.98	kPa	NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	201.40		NIST Webbook
rinpol	199.60		NIST Webbook
rinpol	201.49		NIST Webbook
rinpol	201.49		NIST Webbook
rinpol	201.68		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	201.49		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1198.20		NIST Webbook
rinpol	1196.30		NIST Webbook
rinpol	1195.40		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1166.50		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1165.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2233.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2189.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2233.00		NIST Webbook

tb	500.15 ± 2.00	K	NIST Webbook
tb	498.15 ± 3.00	K	NIST Webbook
tb	500.85 ± 2.00	K	NIST Webbook
tb	499.15 ± 2.00	K	NIST Webbook
tb	500.00	K	KDB
tb	500.20	K	NIST Webbook
tb	498.15 ± 2.00	K	NIST Webbook
tb	498.15 ± 2.00	K	NIST Webbook
tb	500.85 ± 3.00	K	NIST Webbook
tb	500.05 ± 2.00	K	NIST Webbook
tc	729.85 ± 0.80	K	NIST Webbook
tc	769.55 ± 2.00	K	NIST Webbook
tc	729.80	K	KDB
tf	335.90 ± 2.00	K	NIST Webbook
tf	336.15 ± 2.00	K	NIST Webbook
tf	338.45 ± 1.00	K	NIST Webbook
tf	335.65 ± 0.30	K	NIST Webbook
tf	338.23 ± 0.10	K	NIST Webbook
tf	338.15 ± 2.00	K	NIST Webbook
tf	335.15 ± 2.00	K	NIST Webbook
tf	338.15 ± 2.00	K	NIST Webbook
tf	335.65 ± 2.00	K	NIST Webbook
tf	337.45 ± 0.50	K	NIST Webbook
tf	335.15 ± 3.00	K	NIST Webbook
tf	334.15 ± 3.00	K	NIST Webbook
tf	338.15 ± 2.00	K	NIST Webbook
tf	338.26 ± 0.05	K	NIST Webbook
tf	338.15 ± 0.20	K	NIST Webbook
tf	336.75	K	Aqueous Solubility Prediction Method
tf	333.90	K	KDB
tf	341.15	K	Liquid pharmaceuticals formulation by eutectic formation
vc	0.365	m3/kmol	Cheméo Relay (1.0)

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	0.0006876	Pa×s	385.29	Joback Method
dvisc	0.0000891	Pa×s	494.72	Joback Method
dvisc	0.0013928	Pa×s	357.94	Joback Method
dvisc	0.0031710	Pa×s	330.58	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	18.13	kJ/mol	334.00	NIST Webbook
hfust	19.04	kJ/mol	338.50	NIST Webbook
hfust	18.13	kJ/mol	334.00	NIST Webbook
hfust	18.13	kJ/mol	334.00	NIST Webbook
hsubt	85.70 ± 0.10	kJ/mol	302.50	NIST Webbook
hsubt	72.40 ± 0.80	kJ/mol	299.00	NIST Webbook
hvapt	54.90	kJ/mol	473.00	NIST Webbook
sfust	54.27	J/mol×K	334.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54534e+01
Coeff. B	-4.54866e+03
Coeff. C	-8.01920e+01
Temperature range (K), min.	380.12
Temperature range (K), max.	528.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.67166e+02
Coeff. B	-1.46931e+04
Coeff. C	-2.18420e+01
Coeff. D	1.03338e-05
Temperature range (K), min.	338.25
Temperature range (K), max.	729.95

Sources

Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=878
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol878.mol
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
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=C95658&Units=SI

Legend

af:	Acentric Factor
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
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