Phenol, 2,4,6-trimethyl-

Other names:	1-Hydroxy-2,4,6-trimethylbenzene
	2,4,6-TRIMETHYL PHENOL
	2,4,6-Trimethylphenol
	2,4,6-Trimetylofenol
	2-Hydroxymesitylene
	Mesitol
	Mesityl alcohol
Inchi:	InChI=1S/C9H12O/c1-6-4-7(2)9(10)8(3)5-6/h4-5,10H,1-3H3
InchiKey:	BPRYUXCVCCNUFE-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	Cc1cc(C)c(O)c(C)c1
Mol. weight [g/mol]:	136.19
CAS:	527-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-36.57	kJ/mol	Joback Method
hf	-263.70	kJ/mol	NIST Webbook
hf	-176.90	kJ/mol	NIST Webbook
hfus	18.11	kJ/mol	Joback Method
hsub	82.80 ± 0.30	kJ/mol	NIST Webbook
hsub	95.00	kJ/mol	NIST Webbook
hsub	93.10	kJ/mol	NIST Webbook
hsub	95.02	kJ/mol	NIST Webbook
hvap	52.24	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-2.05		Estimated Solubility Method
log10ws	-2.05		Aqueous Solubility Prediction Method
logp	2.317		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1204.10		NIST Webbook
rinpol	1199.10		NIST Webbook
rinpol	1202.50		NIST Webbook

rinpol	1204.10		NIST Webbook
rinpol	1202.50		NIST Webbook
rinpol	1201.60		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1202.50		NIST Webbook
rinpol	1212.90		NIST Webbook
rinpol	1215.80		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1199.10		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	203.83		NIST Webbook
rinpol	202.50		NIST Webbook
rinpol	203.59		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1201.60		NIST Webbook
rinpol	1199.10		NIST Webbook
rinpol	1202.50		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1202.50		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	494.15 ± 3.00	K	NIST Webbook
tc	747.15	K	Joback Method
tf	341.15 ± 4.00	K	NIST Webbook
tf	345.65 ± 2.00	K	NIST Webbook
tf	344.15 ± 2.00	K	NIST Webbook
tf	342.15 ± 2.00	K	NIST Webbook
tf	345.25 ± 2.00	K	NIST Webbook
tf	345.45 ± 1.50	K	NIST Webbook
tf	344.55 ± 2.00	K	NIST Webbook
tf	343.90 ± 2.00	K	NIST Webbook
tf	345.65	K	Aqueous Solubility Prediction Method
tf	343.65 ± 2.00	K	NIST Webbook
tf	346.15	K	Liquid pharmaceuticals formulation by eutectic formation

tf	345.40 ± 3.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.50	J/mol×K	747.15	Joback Method
cpg	266.77	J/mol×K	522.58	Joback Method
cpg	278.94	J/mol×K	560.01	Joback Method
cpg	290.34	J/mol×K	597.44	Joback Method
cpg	301.03	J/mol×K	634.86	Joback Method
cpg	311.07	J/mol×K	672.29	Joback Method
cpg	320.54	J/mol×K	709.72	Joback Method
dvisc	0.0000662	Pa×s	522.58	Joback Method
dvisc	0.0017439	Pa×s	354.37	Joback Method
dvisc	0.0008278	Pa×s	382.40	Joback Method
dvisc	0.0004351	Pa×s	410.44	Joback Method
dvisc	0.0002482	Pa×s	438.47	Joback Method
dvisc	0.0001515	Pa×s	466.51	Joback Method
dvisc	0.0000978	Pa×s	494.54	Joback Method
hvapt	53.20	kJ/mol	430.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54349e+01
Coeff. B	-4.49407e+03
Coeff. C	-7.84680e+01
Temperature range (K), min.	345.15
Temperature range (K), max.	522.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.88733e+01

Coeff. B	-8.88021e+03
Coeff. C	-7.60503e+00
Coeff. D	3.74291e-06
Temperature range (K), min.	367.15
Temperature range (K), max.	494.15

Sources

Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C527606&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermochemistry of Li, Na, K, Rb and Cs alkylated phenoxides:	https://www.doi.org/10.1016/j.tca.2005.02.027
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=881
Solubilities of Substituted Phenols in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060058e
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol881.mol

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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

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

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