Phenol, 2-(1-methylethyl)-

Other names:	1-Hydroxy-2-isopropylbenzene 2-(1-Methylethyl)phenol 2-Isopropylphenol Isopropylphenol, ortho NSC 5103 Phenol, o-isopropyl- Prodox 131 o-Cumenol o-Hydroxycumene o-Isopropylphenol
Inchi:	InChI=1S/C9H12O/c1-7(2)8-5-3-4-6-9(8)10/h3-7,10H,1-2H3
InchiKey:	CRBJBYGJVIBWIY-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CC(C)c1ccccc1O
Mol. weight [g/mol]:	136.19
CAS:	88-69-7

Physical Properties

Property code	Value	Unit	Source
chl	-5022.90	kJ/mol	NIST Webbook
gf	-19.75	kJ/mol	Joback Method
hf	-175.30 ± 2.40	kJ/mol	NIST Webbook
hf	-161.30	kJ/mol	NIST Webbook
hfl	-230.00	kJ/mol	NIST Webbook
hfus	15.37	kJ/mol	Joback Method
hvap	68.70	kJ/mol	NIST Webbook
hvap	73.01	kJ/mol	NIST Webbook
log10ws	-2.20		Crippen Method
logp	2.516		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1199.20		NIST Webbook
rinpol	1200.20		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1200.00		NIST Webbook

rinpol	1198.00		NIST Webbook
rinpol	1198.90		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	203.41		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1198.90		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1175.40		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2111.00		NIST Webbook
tb	512.18	K	Joback Method
tc	739.56	K	Joback Method
tf	288.65 ± 2.00	K	NIST Webbook
tf	290.00 ± 0.20	K	NIST Webbook
tf	288.65 ± 2.00	K	NIST Webbook
tf	288.65 ± 2.00	K	NIST Webbook
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.53	J/mol×K	512.18	Joback Method
cpg	280.87	J/mol×K	550.08	Joback Method
cpg	293.23	J/mol×K	587.97	Joback Method
cpg	304.71	J/mol×K	625.87	Joback Method
cpg	315.38	J/mol×K	663.76	Joback Method
cpg	325.34	J/mol×K	701.66	Joback Method
cpg	334.65	J/mol×K	739.56	Joback Method
dvisc	0.0009146	Pa×s	380.28	Joback Method
dvisc	0.0023278	Pa×s	347.31	Joback Method
dvisc	0.0072081	Pa×s	314.33	Joback Method
dvisc	0.0004171	Pa×s	413.25	Joback Method
dvisc	0.0002136	Pa×s	446.23	Joback Method
dvisc	0.0001200	Pa×s	479.21	Joback Method
dvisc	0.0000726	Pa×s	512.18	Joback Method
hvapt	63.50	kJ/mol	434.00	NIST Webbook
hvapt	55.10	kJ/mol	429.50	NIST Webbook

hvapt	56.10	kJ/mol	434.00	NIST Webbook
hvapt	57.30	kJ/mol	418.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54296e+01
Coeff. B	-4.44272e+03
Coeff. C	-7.67170e+01
Temperature range (K), min.	370.12
Temperature range (K), max.	515.80

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88697&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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