p-Cumenol

Other names:	1-Hydroxy-4-isopropylbenzene
	4-(1-Methylethyl)phenol
	4-Isopropylphenol
	Australol
	NSC 1888
	Phenol, 4-(1-methylethyl)-
	Phenol, p-isopropyl-
	Prodox 133
	p-Cuminol
	p-Isopropylphenol
Inchi:	InChI=1S/C9H12O/c1-7(2)8-3-5-9(10)6-4-8/h3-7,10H,1-2H3
InchiKey:	YQUQWHNMBPIWGK-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CC(C)c1ccc(O)cc1
Mol. weight [g/mol]:	136.19
CAS:	99-89-8

Physical Properties

Property code	Value	Unit	Source
chs	-4983.00	kJ/mol	NIST Webbook
chs	-4977.00 ± 13.00	kJ/mol	NIST Webbook
gf	-19.75	kJ/mol	Joback Method
hf	-175.30 ± 2.40	kJ/mol	NIST Webbook
hf	-183.90	kJ/mol	NIST Webbook
hfs	-270.00	kJ/mol	NIST Webbook
hfus	15.37	kJ/mol	Joback Method
hsub	86.10	kJ/mol	NIST Webbook
hsub	88.07	kJ/mol	NIST Webbook
hvap	50.53	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.516		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1227.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1221.00		NIST Webbook

rinpol	1247.00		NIST Webbook
rinpol	206.10		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	206.10		NIST Webbook
ripol	2243.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2242.00		NIST Webbook
tb	502.45 ± 3.00	K	NIST Webbook
tb	503.15 ± 3.00	K	NIST Webbook
tb	500.15 ± 3.00	K	NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook
tb	497.15 ± 3.00	K	NIST Webbook
tb	485.50	K	NIST Webbook
tb	496.20 ± 1.00	K	NIST Webbook
tb	501.65 ± 3.00	K	NIST Webbook
tb	497.15 ± 3.00	K	NIST Webbook
tb	500.15 ± 3.00	K	NIST Webbook
tb	502.25 ± 3.00	K	NIST Webbook
tb	501.35 ± 3.00	K	NIST Webbook
tb	500.15 ± 4.00	K	NIST Webbook
tc	739.56	K	Joback Method
tf	334.15 ± 2.00	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
tf	332.00 ± 2.00	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
tf	335.15 ± 2.00	K	NIST Webbook
tf	335.15 ± 2.00	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
tf	333.15 ± 2.00	K	NIST Webbook
tf	336.20 ± 0.20	K	NIST Webbook
tf	334.15 ± 2.00	K	NIST Webbook
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.38	J/mol×K	663.76	Joback Method
cpg	334.65	J/mol×K	739.56	Joback Method
cpg	325.34	J/mol×K	701.66	Joback Method
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
dvisc	0.0000726	Pa×s	512.18	Joback Method
dvisc	0.0002136	Pa×s	446.23	Joback Method
dvisc	0.0001200	Pa×s	479.21	Joback Method
dvisc	0.0072081	Pa×s	314.33	Joback Method
dvisc	0.0023278	Pa×s	347.31	Joback Method
dvisc	0.0009146	Pa×s	380.28	Joback Method
dvisc	0.0004171	Pa×s	413.25	Joback Method
hsubt	56.00 ± 2.00	kJ/mol	223.00	NIST Webbook
hvapt	63.10	kJ/mol	438.00	NIST Webbook
hvapt	63.70	kJ/mol	449.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54416e+01
Coeff. B	-4.56253e+03
Coeff. C	-8.08030e+01
Temperature range (K), min.	381.88
Temperature range (K), max.	531.19

Sources

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=C99898&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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