Phenol, 4-(1-methyl-1-phenylethyl)-

Other names: 2-Phenyl-2-(4-hydroxyphenyl)propane
2-Phenyl-2-(p-hydroxyphenyl)propane
4-(1-METHYL-1-PHENYLETHYL)PHENOL
4-(2-Phenylisopropyl) phenol
4-(ALPHA,ALPHA-DIMETHYLBENZYL)PHENOL
4-(Dimethylphenylmethyl)phenol
4-(«alpha»,«alpha»-Dimethylbenzyl)phenol
4-(Â«alphaÂ»,Â«alphaÂ»-Dimethylbenzyl)phenol
4-Cumylphenol
4-Hydroxydiphenyldimethylmethane
NSC 6237
P-ALPHA-CUMYLPHENOL
Phenol, 4-(1-methyl-1-phenethyl)-
Phenol, p-(«alpha»,«alpha»-dimethylbenzyl)-
Phenol, p-(Â«alphaÂ»,Â«alphaÂ»-dimethylbenzyl)-
p-(«alpha»,«alpha»-Dimethylbenzyl)phenol
p-(«alpha»-Cumyl)phenol
p-(Â«alphaÂ»,Â«alphaÂ»-Dimethylbenzyl)phenol
p-(Â«alphaÂ»-Cumyl)phenol
p-.alpha.-Cumylphenol
p-Cumylphenol
p-Hydroxy-2,2-diphenylpropane

Inchi: InChI=1S/C15H16O/c1-15(2,12-6-4-3-5-7-12)13-8-10-14(16)11-9-13/h3-11,16H,1-2H3

InchiKey: QBDSZLJBMIMQRS-UHFFFAOYSA-N

Formula: C15H16O

SMILES: CC(C)(c1ccccc1)c1ccc(O)cc1

Mol. weight [g/mol]: 212.29

CAS: 599-64-4

Physical Properties

Property code	Value	Unit	Source
gf	148.46	kJ/mol	Joback Method
hf	-65.93	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method

logp	3.718		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1860.00		NIST Webbook
tb	608.20	K	NIST Webbook
tc	931.82	K	Joback Method
tf	346.40 ± 0.05	K	NIST Webbook
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.34	J/mol×K	673.35	Joback Method
cpg	496.80	J/mol×K	716.43	Joback Method
cpg	511.88	J/mol×K	759.51	Joback Method
cpg	525.77	J/mol×K	802.58	Joback Method
cpg	538.68	J/mol×K	845.66	Joback Method
cpg	550.83	J/mol×K	888.74	Joback Method
cpg	562.39	J/mol×K	931.82	Joback Method
dvisc	0.0002905	Pa×s	467.05	Joback Method
dvisc	0.0007455	Pa×s	425.79	Joback Method
dvisc	0.0001319	Pa×s	508.31	Joback Method
dvisc	0.0000674	Pa×s	549.57	Joback Method
dvisc	0.0000379	Pa×s	590.83	Joback Method
dvisc	0.0000229	Pa×s	632.09	Joback Method
dvisc	0.0000148	Pa×s	673.35	Joback Method
hfust	21.68	kJ/mol	346.40	NIST Webbook
hfust	22.80	kJ/mol	346.20	NIST Webbook
hfust	21.68	kJ/mol	346.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53045e+01
Coeff. B	-5.46100e+03
Coeff. C	-9.71150e+01

Temperature range (K), min.	460.77
Temperature range (K), max.	643.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.07084e+02
Coeff. B	-1.41369e+04
Coeff. C	-1.25239e+01
Coeff. D	2.83679e-06
Temperature range (K), min.	346.00
Temperature range (K), max.	834.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C599644&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=889

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

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol889.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

hfust: Enthalpy of fusion at a given temperature

hvap: Enthalpy of vaporization at standard conditions

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