Phenol, 4-(1,1-dimethylpropyl)-

Other names:	1-Hydroxy-4-(1,1-dimethylpropyl)benzene
	1-Hydroxy-4-(2-methyl-2-butyl)benzene
	2-Methyl-2-p-hydroxyphenylbutane
	4-(1,1-Dimethylpropyl)-1-phenol
	4-(1,1-Dimethylpropyl)Phenol
	4-t-Amylphenol
	4-tert-Amylphenol
	4-tert-Pentylphenol
	AMILFENOL
	Amilphenol
	Amyl phenol 4T
	NSC 403672
	Nipacide PTAP
	P-(ALPHA,ALPHA-DIMETHYLPROPYL)PHENOL
	P-TERT-AMYLPHENOL
	P-TERT-PENTYLPHENOL
	PTAP
	Para-tertiary amylphenol
	Pentaphen
	Pentaphen 67
	Phenol, p-tert-pentyl-
	Ucar amyl phenol 4T
	p-(1,1-Dimethyl propyl) phenol
	p-(«alpha»,«alpha»-Dimethylpropyl)phenol
	p-(Â«alphaÂ»,Â«alphaÂ»-Dimethylpropyl)phenol
	p-t-Amyl phenol
	p-t-Pentylphenol
Inchi:	InChI=1S/C11H16O/c1-4-11(2,3)9-5-7-10(12)8-6-9/h5-8,12H,4H2,1-3H3
InchiKey:	NRZWYNLTFLDQQX-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCC(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	164.24
CAS:	80-46-6

Physical Properties

Property code	Value	Unit	Source

gf	2.37	kJ/mol	Joback Method
hf	-219.90	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hsub	88.30 ± 0.50	kJ/mol	NIST Webbook
hvap	65.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.75		Crippen Method
logp	3.080		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1404.40		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1397.20		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1400.10		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1417.00		NIST Webbook
tb	528.20	K	NIST Webbook
tb	535.65 ± 4.00	K	NIST Webbook
tc	783.63	K	Joback Method
tf	366.15 ± 2.00	K	NIST Webbook
tf	368.00 ± 3.00	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.68	J/mol×K	707.47	Joback Method
cpg	439.00	J/mol×K	783.63	Joback Method
cpg	428.20	J/mol×K	745.55	Joback Method
cpg	360.99	J/mol×K	555.15	Joback Method
cpg	376.58	J/mol×K	593.23	Joback Method
cpg	390.98	J/mol×K	631.31	Joback Method
cpg	404.31	J/mol×K	669.39	Joback Method
dvisc	0.0000453	Pa×s	555.15	Joback Method
dvisc	0.0001257	Pa×s	488.20	Joback Method
dvisc	0.0000730	Pa×s	521.67	Joback Method
dvisc	0.0030819	Pa×s	354.29	Joback Method
dvisc	0.0011258	Pa×s	387.77	Joback Method
dvisc	0.0004826	Pa×s	421.24	Joback Method
dvisc	0.0002344	Pa×s	454.72	Joback Method

hsubt	87.40 ± 0.50	kJ/mol	313.00	NIST Webbook
hvapt	58.20	kJ/mol	466.50	NIST Webbook
hvapt	64.20 ± 0.20	kJ/mol	315.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61421e+01
Coeff. B	-5.04901e+03
Coeff. C	-9.00610e+01
Temperature range (K), min.	408.52
Temperature range (K), max.	556.24

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.16689e+02
Coeff. B	-1.25669e+04
Coeff. C	-1.43529e+01
Coeff. D	5.47644e-06
Temperature range (K), min.	366.00
Temperature range (K), max.	751.00

Sources

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

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=887

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80466&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=887

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

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