Phenol, 2-(1,1-dimethylethyl)-4-methyl-

Other names:	1-Hydroxy-2-tert-butyl-4-methylbenzene
	2-(1,1'-dimethylethyl)-4-methylphenol
	2-(1,1-Dimethylethyl)-4-methyl-phenol
	2-Terc.butyl-p-kresol
	2-t-Butyl-4-methylphenol
	2-t-Butyl-p-cresol
	2-tert-Butyl-4-Methylphenol
	2-tert-Butyl-4-cresol
	2-tert-Butyl-4-methyl-1-phenol
	2-tert-Butyl-p-Cresol
	4-Methyl-2-(1,1-dimethylethyl)phenol
	4-Methyl-2-tert-butylphenol
	4-Methyl-6-t-butylphenol
	NSC 60301
	o-tert-Butyl-p-cresol
	p-Cresol, 2-tert-butyl-
Inchi:	InChI=1S/C11H16O/c1-8-5-6-10(12)9(7-8)11(2,3)4/h5-7,12H,1-4H3
InchiKey:	IKEHOXWJQXIQAG-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	Cc1ccc(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	164.24
CAS:	2409-55-4

Physical Properties

Property code	Value	Unit	Source
gf	-7.26	kJ/mol	Joback Method
hf	-207.00 ± 3.20	kJ/mol	NIST Webbook
hfus	16.27	kJ/mol	Joback Method
hsub	82.90 ± 0.50	kJ/mol	NIST Webbook
hvap	65.70 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.81		Crippen Method
logp	2.998		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1352.20		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1353.10		NIST Webbook

rinpol	1387.00		NIST Webbook
rinpol	1352.20		NIST Webbook
rinpol	1345.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		NIST Webbook
tb	510.20	K	NIST Webbook
tc	789.71	K	Joback Method
tf	325.16 ± 0.30	K	NIST Webbook
tf	325.45 ± 0.20	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.74	J/mol×K	560.13	Joback Method
cpg	375.98	J/mol×K	598.39	Joback Method
cpg	390.09	J/mol×K	636.66	Joback Method
cpg	403.20	J/mol×K	674.92	Joback Method
cpg	415.40	J/mol×K	713.18	Joback Method
cpg	426.81	J/mol×K	751.44	Joback Method
cpg	437.54	J/mol×K	789.71	Joback Method
dvisc	0.0000425	Pa×s	560.13	Joback Method
dvisc	0.0008050	Pa×s	399.03	Joback Method
dvisc	0.0003749	Pa×s	431.25	Joback Method
dvisc	0.0001942	Pa×s	463.47	Joback Method
dvisc	0.0019771	Pa×s	366.81	Joback Method
dvisc	0.0000663	Pa×s	527.91	Joback Method
dvisc	0.0001095	Pa×s	495.69	Joback Method
hsubt	82.60 ± 0.50	kJ/mol	303.00	NIST Webbook
hsubt	77.40	kJ/mol	284.00	NIST Webbook
hvapt	63.00 ± 0.30	kJ/mol	342.50	NIST Webbook
hvapt	58.90	kJ/mol	451.00	NIST Webbook
hvapt	57.70	kJ/mol	425.00	NIST Webbook
hvapt	55.70	kJ/mol	425.00	NIST Webbook
hvapt	52.60	kJ/mol	425.00	NIST Webbook
hvapt	48.50	kJ/mol	425.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44886e+01
Coeff. B	-4.33342e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	388.12
Temperature range (K), max.	555.17

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2409554&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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