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

Other names:	2-Methyl-4-tert-butylphenol
	4-tert-Butyl-2-Methylphenol
	4-tert-Butyl-o-Cresol
	Phenol, 4-tert-butyl-2-methyl-
	o-Cresol, 4-tert-butyl-
	p-tert-Butyl-o-cresol
Inchi:	InChI=1S/C11H16O/c1-8-7-9(11(2,3)4)5-6-10(8)12/h5-7,12H,1-4H3
InchiKey:	SNKLPZOJLXDZCW-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	Cc1cc(C(C)(C)C)ccc1O
Mol. weight [g/mol]:	164.24
CAS:	98-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-7.26	kJ/mol	Joback Method
hf	-231.37	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	72.10 ± 0.60	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	1333.60		NIST Webbook
tb	560.13	K	Joback Method
tc	789.71	K	Joback Method
tf	366.81	K	Joback Method
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	437.54	J/mol×K	789.71	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	375.98	J/mol×K	598.39	Joback Method
dvisc	0.0000663	Pa×s	527.91	Joback Method
dvisc	0.0001095	Pa×s	495.69	Joback Method
dvisc	0.0001942	Pa×s	463.47	Joback Method
dvisc	0.0003749	Pa×s	431.25	Joback Method
dvisc	0.0008050	Pa×s	399.03	Joback Method
dvisc	0.0000425	Pa×s	560.13	Joback Method
dvisc	0.0019771	Pa×s	366.81	Joback Method
hvapt	46.70	kJ/mol	439.50	NIST Webbook
hvapt	50.90	kJ/mol	439.50	NIST Webbook
hvapt	53.20	kJ/mol	439.50	NIST Webbook
hvapt	55.70	kJ/mol	439.50	NIST Webbook
hvapt	75.70	kJ/mol	286.00	NIST Webbook
hvapt	61.50	kJ/mol	433.50	NIST Webbook
hvapt	71.30 ± 0.60	kJ/mol	312.00	NIST Webbook
hvapt	53.90	kJ/mol	439.50	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

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=C98271&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

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
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