Phenol, m-tert-butyl-

Other names:	3-t-Butylphenol
	3-tert-Butylphenol
	Phenol, 3-(1,1-dimethylethyl)-
	Phenol, 3-tert-butyl-
	m-tert-Butylphenol
Inchi:	InChI=1S/C10H14O/c1-10(2,3)8-5-4-6-9(11)7-8/h4-7,11H,1-3H3
InchiKey:	CYEKUDPFXBLGHH-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)(C)c1cccc(O)c1
Mol. weight [g/mol]:	150.22
CAS:	585-34-2

Physical Properties

Property code	Value	Unit	Source
chs	-5661.00	kJ/mol	NIST Webbook
gf	-6.05	kJ/mol	Joback Method
hf	-185.20	kJ/mol	NIST Webbook
hf	-184.00	kJ/mol	NIST Webbook
hfs	-280.00	kJ/mol	NIST Webbook
hfus	14.07	kJ/mol	Joback Method
hsub	96.00	kJ/mol	NIST Webbook
hsub	86.00 ± 0.50	kJ/mol	NIST Webbook
hsub	92.05	kJ/mol	NIST Webbook
hsub	88.90 ± 0.50	kJ/mol	NIST Webbook
hvap	71.30 ± 0.80	kJ/mol	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.690		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1294.70		NIST Webbook
rinpol	1294.70		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1296.70		NIST Webbook
rinpol	1294.80		NIST Webbook
tb	532.27	K	Joback Method

tc	765.16	K	Joback Method
tf	343.02	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.96	J/mol×K	532.27	Joback Method
cpg	329.85	J/mol×K	571.08	Joback Method
cpg	343.53	J/mol×K	609.90	Joback Method
cpg	356.13	J/mol×K	648.71	Joback Method
cpg	367.75	J/mol×K	687.53	Joback Method
cpg	378.53	J/mol×K	726.34	Joback Method
cpg	388.58	J/mol×K	765.16	Joback Method
dvisc	0.0000583	Pa×s	532.27	Joback Method
dvisc	0.0014227	Pa×s	374.56	Joback Method
dvisc	0.0006157	Pa×s	406.10	Joback Method
dvisc	0.0038345	Pa×s	343.02	Joback Method
dvisc	0.0001617	Pa×s	469.19	Joback Method
dvisc	0.0000940	Pa×s	500.73	Joback Method
dvisc	0.0003007	Pa×s	437.64	Joback Method
hsubt	70.70	kJ/mol	282.50	NIST Webbook
hvapt	69.10 ± 0.80	kJ/mol	334.00	NIST Webbook
hvapt	62.40	kJ/mol	457.50	NIST Webbook
hvapt	56.60	kJ/mol	457.50	NIST Webbook
hvapt	54.40	kJ/mol	457.50	NIST Webbook
hvapt	49.90	kJ/mol	457.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54501e+01
Coeff. B	-4.65055e+03
Coeff. C	-8.38060e+01
Temperature range (K), min.	390.52
Temperature range (K), max.	542.50

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C585342&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ie:	Ionization energy
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

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