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

Other names:	2-(1,1-Dimethylethyl)-phenol
	2-(1,1-dimethylethyl)phenol
	2-t-Butylphenol
	2-tert-Butylphenol
	2-tert-butyl-1-hydroxybenzene
	Phenol, 2-tert-butyl-
	Phenol, o-tert-butyl-
	o-tert-Butylphenol
Inchi:	InChI=1S/C10H14O/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7,11H,1-3H3
InchiKey:	WJQOZHYUIDYNHM-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)(C)c1ccccc1O
Mol. weight [g/mol]:	150.22
CAS:	88-18-6

Physical Properties

Property code	Value	Unit	Source
chl	-5660.10	kJ/mol	NIST Webbook
gf	-6.05	kJ/mol	Joback Method
hf	-199.10	kJ/mol	NIST Webbook
hfl	-280.00	kJ/mol	NIST Webbook
hfus	14.07	kJ/mol	Joback Method
hvap	63.20 ± 0.20	kJ/mol	NIST Webbook
hvap	80.90	kJ/mol	NIST Webbook
hvap	77.03	kJ/mol	NIST Webbook
ie	8.10 ± 0.02	eV	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	1273.20		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1274.90		NIST Webbook
rinpol	1249.00		NIST Webbook

rinpol	1250.00		NIST Webbook
rinpol	1273.50		NIST Webbook
ripol	2161.00		NIST Webbook
ripol	2161.00		NIST Webbook
tb	497.06 ± 0.01	K	NIST Webbook
tb	497.20	K	NIST Webbook
tc	765.16	K	Joback Method
tf	267.53 ± 0.05	K	NIST Webbook
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	388.58	J/mol×K	765.16	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	329.85	J/mol×K	571.08	Joback Method
dvisc	0.0000940	Pa×s	500.73	Joback Method
dvisc	0.0001617	Pa×s	469.19	Joback Method
dvisc	0.0003007	Pa×s	437.64	Joback Method
dvisc	0.0006157	Pa×s	406.10	Joback Method
dvisc	0.0014227	Pa×s	374.56	Joback Method
dvisc	0.0000583	Pa×s	532.27	Joback Method
dvisc	0.0038345	Pa×s	343.02	Joback Method
hvapt	47.00	kJ/mol	418.50	NIST Webbook
hvapt	51.00	kJ/mol	418.50	NIST Webbook
hvapt	53.90	kJ/mol	418.50	NIST Webbook
hvapt	52.90	kJ/mol	437.00	NIST Webbook
hvapt	54.90	kJ/mol	425.50	NIST Webbook
hvapt	74.10	kJ/mol	438.00	NIST Webbook
hvapt	62.60 ± 0.20	kJ/mol	309.00	NIST Webbook
hvapt	55.60	kJ/mol	418.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	418.50	K	9.90	Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component
tbp	438.60	K	19.82	Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component
tbp	451.70	K	29.75	Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component
tbp	469.40	K	49.63	Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component
tbp	479.20	K	64.61	Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54375e+01
Coeff. B	-4.52080e+03
Coeff. C	-7.93800e+01
Temperature range (K), min.	377.78
Temperature range (K), max.	525.83

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component:	https://www.doi.org/10.1016/j.tca.2016.05.011
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=C88186&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

Legend

chl:	Standard liquid 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
hfl:	Liquid phase 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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume