Phenol, 2-(1,1-dimethylethyl)-5-methyl-

Other names:	2-t-Butyl-5-methylphenol
	2-tert-Butyl-5-Methylphenol
	3-Methyl-6-tert-butylphenol
	5-Methyl-2-(1,1-dimethylethyl)-phenol
	6-tert-Butyl-3-Methylphenol
	6-tert-Butyl-m-Cresol
	m-Cresol, 6-tert-butyl-
Inchi:	InChI=1S/C11H16O/c1-8-5-6-9(10(12)7-8)11(2,3)4/h5-7,12H,1-4H3
InchiKey:	XOUQAVYLRNOXDO-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	Cc1ccc(C(C)(C)C)c(O)c1
Mol. weight [g/mol]:	164.24
CAS:	88-60-8

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
hsub	79.70 ± 1.30	kJ/mol	NIST Webbook
hvap	67.20 ± 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	1340.40		NIST Webbook
rinpol	1365.40		NIST Webbook
rinpol	1366.40		NIST Webbook
rinpol	1368.50		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	560.13	K	Joback Method
tc	789.71	K	Joback Method
tf	294.20 ± 0.50	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.40	J/mol×K	713.18	Joback Method
cpg	437.54	J/mol×K	789.71	Joback Method
cpg	426.81	J/mol×K	751.44	Joback Method
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
dvisc	0.0001095	Pa×s	495.69	Joback Method
dvisc	0.0000663	Pa×s	527.91	Joback Method
dvisc	0.0000425	Pa×s	560.13	Joback Method
dvisc	0.0019771	Pa×s	366.81	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
hsubt	80.40 ± 1.30	kJ/mol	285.50	NIST Webbook
hvapt	53.00	kJ/mol	450.50	NIST Webbook
hvapt	59.80	kJ/mol	434.00	NIST Webbook
hvapt	65.90 ± 0.30	kJ/mol	319.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	1.60	NIST Webbook
tbrp	400.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44773e+01

Coeff. B	-4.32884e+03
Coeff. C	-8.29300e+01
Temperature range (K), min.	388.00
Temperature range (K), max.	555.21

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=C88608&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume