Phenol, 2-(1-methylpropyl)-

Other names:	2-(1-Methylpropyl)phenol
	2-sec-Butylphenol
	2-sec.Butylfenol
	Phenol, o-sec-butyl-
	o-sec-Butylphenol
Inchi:	InChI=1S/C10H14O/c1-3-8(2)9-6-4-5-7-10(9)11/h4-8,11H,3H2,1-2H3
InchiKey:	NGFPWHGISWUQOI-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCC(C)c1ccccc1O
Mol. weight [g/mol]:	150.22
CAS:	89-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-11.33	kJ/mol	Joback Method
hf	-191.40	kJ/mol	NIST Webbook
hfl	-251.30	kJ/mol	NIST Webbook
hfus	17.96	kJ/mol	Joback Method
hvap	59.90	kJ/mol	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.906		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	500.65 ± 3.00	K	NIST Webbook
tb	503.65 ± 4.00	K	NIST Webbook
tb	496.15 ± 3.00	K	NIST Webbook
tb	500.15 ± 3.00	K	NIST Webbook
tb	500.20	K	NIST Webbook
tb	500.65 ± 3.00	K	NIST Webbook
tc	758.39	K	Joback Method
tf	291.15 ± 3.00	K	NIST Webbook
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.11	J/mol×K	758.39	Joback Method
cpg	373.98	J/mol×K	721.17	Joback Method
cpg	363.20	J/mol×K	683.95	Joback Method
cpg	351.67	J/mol×K	646.73	Joback Method
cpg	339.34	J/mol×K	609.50	Joback Method
cpg	326.10	J/mol×K	572.28	Joback Method
cpg	311.88	J/mol×K	535.06	Joback Method
dvisc	0.0057625	Pa×s	325.60	Joback Method
dvisc	0.0000572	Pa×s	535.06	Joback Method
dvisc	0.0000944	Pa×s	500.15	Joback Method
dvisc	0.0001678	Pa×s	465.24	Joback Method
dvisc	0.0003276	Pa×s	430.33	Joback Method
dvisc	0.0007197	Pa×s	395.42	Joback Method
dvisc	0.0018414	Pa×s	360.51	Joback Method
hvapt	52.10	kJ/mol	482.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54407e+01
Coeff. B	-4.55275e+03
Coeff. C	-8.04700e+01
Temperature range (K), min.	380.92
Temperature range (K), max.	529.94

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=C89725&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
Mutual Solubilities for the Water 2-sec-Butylphenol System and Partition Coefficients for Furfural and Formic Acid in the Water 2-sec-Butylphenol System:	https://www.doi.org/10.1021/acs.jced.5b00170

Legend

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
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