Benzoic acid, p-tert-butyl-

Other names:	4-(1,1-Dimethylethyl)benzoic acid
	4-t-Butylbenzoic acid
	4-tert-Butylbenzoic acid
	Benzoic acid, 4-(1,1-dimethylethyl)-
	Kyselina p-terc.butylbenzoova
	NSC 4802
	TBBA
	benzoic acid, 4-(1,1,-dimethylethyl)-
	benzoic aid, p-tert-butyl-
	p-t-Butylbenzoic acid
	p-tert-Butylbenzoic acid
Inchi:	InChI=1S/C11H14O2/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h4-7H,1-3H3,(H,12,13)
InchiKey:	KDVYCTOWXSLNNI-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(C)(C)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	178.23
CAS:	98-73-7

Physical Properties

Property code	Value	Unit	Source
chs	-5826.57 ± 0.90	kJ/mol	NIST Webbook
gf	-118.38	kJ/mol	Joback Method
hf	-398.50 ± 2.00	kJ/mol	NIST Webbook
hfs	-502.90 ± 1.70	kJ/mol	NIST Webbook
hfus	16.17	kJ/mol	Joback Method
hsub	104.40	kJ/mol	NIST Webbook
hvap	65.15	kJ/mol	Joback Method
ie	8.94 ± 0.02	eV	NIST Webbook
ie	8.94	eV	NIST Webbook
log10ws	-2.85		Crippen Method
logp	2.682		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	625.56	K	Joback Method
tc	834.96	K	Joback Method

tf	438.50 ± 1.00	K	NIST Webbook
tf	438.45 ± 0.50	K	NIST Webbook
tf	436.70 ± 0.00	K	NIST Webbook
tf	439.06	K	Measurement and Modeling of Solubility of para-tert-Butylbenzoic Acid in Pure and Mixed Organic Solvents at Different Temperatures
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.83	J/mol×K	800.06	Joback Method
cpg	440.50	J/mol×K	834.96	Joback Method
cpg	378.05	J/mol×K	625.56	Joback Method
cpg	390.37	J/mol×K	660.46	Joback Method
cpg	401.85	J/mol×K	695.36	Joback Method
cpg	412.56	J/mol×K	730.26	Joback Method
cpg	422.54	J/mol×K	765.16	Joback Method
dvisc	0.0001021	Pa×s	582.27	Joback Method
dvisc	0.0000671	Pa×s	625.56	Joback Method
dvisc	0.0037049	Pa×s	365.84	Joback Method
dvisc	0.0013330	Pa×s	409.13	Joback Method
dvisc	0.0005832	Pa×s	452.41	Joback Method
dvisc	0.0002948	Pa×s	495.70	Joback Method
dvisc	0.0001663	Pa×s	538.99	Joback Method
hfust	17.91	kJ/mol	440.00	NIST Webbook
hfust	17.91	kJ/mol	440.00	NIST Webbook
hsubt	103.80 ± 0.40	kJ/mol	334.00	NIST Webbook
hsubt	104.40 ± 1.00	kJ/mol	334.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30427e+01
Coeff. B	-4.12031e+03

Coeff. C	-8.87680e+01
Temperature range (K), min.	411.80
Temperature range (K), max.	621.71

Sources

Determination and modeling of aqueous solubility of 4-position substituted benzoic acid compounds in a high-temperature solution:	https://www.doi.org/10.1016/j.fluid.2012.11.023
Measurement and Modeling of Solubility of para-tert-Butylbenzoic Acid in Pure and Mixed Organic Solvents at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.6b00965
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination, Correlation, and Application of Sodium l-Ascorbate Solubility in Nine Pure Solvents and Two Binary Solvents at Temperatures from 278.15 to 323.15 K:	https://www.doi.org/10.1021/acs.jced.7b00846
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98737&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and Modeling of Solid Liquid Equilibrium of para-tert-Butylbenzoic Acid in Acetic Acid/Methanol + Water and Acetic Acid + para-tert-Butyltoluene Binary Systems at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.6b00464

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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