

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
mvol	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	438.45 ± 0.50	K	NIST Webbook
tf	438.50 ± 1.00	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	m ³ /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	Paxs	582.27	Joback Method
dvisc	0.0000671	Paxs	625.56	Joback Method
dvisc	0.0037049	Paxs	365.84	Joback Method
dvisc	0.0013330	Paxs	409.13	Joback Method
dvisc	0.0005832	Paxs	452.41	Joback Method
dvisc	0.0002948	Paxs	495.70	Joback Method
dvisc	0.0001663	Paxs	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	$\ln(P_{vp}) = A + B/(T + C)$
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, Correlation, and Application of Sodium L-Ascorbate	https://www.doi.org/10.1021/acs.jced.7b00846
Measurement and Modeling of Solid-Liquid Equilibria of Acetic Acid	https://www.doi.org/10.1021/acs.jced.6b00464
Temperature Dependence of the Solubility of 4-nonylphenol in Acetic Acid	https://www.doi.org/10.1016/j.fluid.2012.11.023
Water Solubility of para-tert-Butylbenzoic Acid	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of para-tert-Butylbenzoic Acid in Water at Different Temperatures	https://www.doi.org/10.1021/acs.jced.6b00965
Measurement and Modeling of Solubility of para-tert-Butylbenzoic Acid in Water at Different Temperatures: Crippen Method	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
NIST Webbook:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98737&Units=SI
	http://link.springer.com/article/10.1007/BF02311772

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

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