

Methyl 4-tert-butylbenzoate

Other names:	4-Tert-butylbenzoic acid methyl ester Benzoic acid, 4-(1,1-dimethylethyl)-, methyl ester Benzoic acid, p-tert-butyl-, methyl ester methyl 4-(1,1-dimethylethyl)benzoate methyl p-tert-butylbenzoate
Inchi:	InChI=1S/C12H16O2/c1-12(2,3)10-7-5-9(6-8-10)11(13)14-4/h5-8H,1-4H3
InchiKey:	UPIJOAFHOIWPLT-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	COC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	192.25
CAS:	26537-19-9

Physical Properties

Property code	Value	Unit	Source
affp	867.10	kJ/mol	NIST Webbook
basg	836.20	kJ/mol	NIST Webbook
gf	-78.14	kJ/mol	Joback Method
hf	-319.50	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
ie	9.38	eV	NIST Webbook
log10ws	-3.03		Crippen Method
logp	2.771		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
tb	578.68	K	Joback Method
tc	798.32	K	Joback Method
tf	338.52	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.08	J/mol×K	578.68	Joback Method
cpg	412.88	J/mol×K	615.29	Joback Method
cpg	427.67	J/mol×K	651.89	Joback Method
cpg	441.50	J/mol×K	688.50	Joback Method
cpg	454.39	J/mol×K	725.10	Joback Method
cpg	466.41	J/mol×K	761.71	Joback Method
cpg	477.58	J/mol×K	798.32	Joback Method
dvisc	0.0019665	Paxs	338.52	Joback Method
dvisc	0.0010426	Paxs	378.55	Joback Method
dvisc	0.0006241	Paxs	418.57	Joback Method
dvisc	0.0004086	Paxs	458.60	Joback Method
dvisc	0.0002864	Paxs	498.63	Joback Method
dvisc	0.0002116	Paxs	538.65	Joback Method
dvisc	0.0001630	Paxs	578.68	Joback Method
pvap	8.53	kPa	448.20	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	1.89	kPa	408.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	2.13	kPa	411.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	3.19	kPa	421.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	4.51	kPa	430.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	5.32	kPa	434.90	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	6.53	kPa	440.60	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	7.93	kPa	446.10	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	1.21	kPa	398.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	9.87	kPa	452.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	10.53	kPa	454.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	11.60	kPa	457.20	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	12.61	kPa	459.70	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	13.87	kPa	462.60	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	14.67	kPa	464.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	15.67	kPa	466.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	16.13	kPa	467.20	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	18.00	kPa	470.70	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	19.73	kPa	473.60	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	20.67	kPa	475.10	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	22.53	kPa	477.90	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	24.13	kPa	480.10	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	25.87	kPa	482.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	26.53	kPa	483.30	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	27.88	kPa	484.90	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	29.13	kPa	486.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	30.40	kPa	487.90	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	31.86	kPa	489.50	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

pvap	32.93	kPa	490.60	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate
pvap	34.66	kPa	492.40	Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate	https://www.doi.org/10.1021/acs.jced.6b00470
Measurement and Correlation Studies of the Saturated Vapor Pressure, Density, Refractive Indices, and Viscosity of Methyl 4-tert-Butylbenzoate	https://www.doi.org/10.1021/acs.jced.6b00965
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=C26537199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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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