

Benzoic acid 1,1-dimethylethyl ester

Other names:	tert-Butyl benzoate Benzoic acid tert-butyl ester Trimethylcarbinol benzoate 1,1-dimethylethyl benzoate
Inchi:	InChI=1S/C11H14O2/c1-11(2,3)13-10(12)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	LYDRKKWPKKEMNZ-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(C)(C)OC(=O)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	774-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-76.93	kJ/mol	Joback Method
hf	-287.39	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.642		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	550.82	K	Joback Method
tc	773.39	K	Joback Method
tf	314.73	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.74	J/mol×K	550.82	Joback Method
cpg	365.17	J/mol×K	587.91	Joback Method
cpg	379.55	J/mol×K	625.01	Joback Method
cpg	392.95	J/mol×K	662.10	Joback Method
cpg	405.40	J/mol×K	699.20	Joback Method

cpg	416.95	J/mol×K	736.29	Joback Method
cpg	427.65	J/mol×K	773.39	Joback Method
dvisc	0.0027809	Pa×s	314.73	Joback Method
dvisc	0.0013780	Pa×s	354.08	Joback Method
dvisc	0.0007858	Pa×s	393.43	Joback Method
dvisc	0.0004963	Pa×s	432.77	Joback Method
dvisc	0.0003384	Pa×s	472.12	Joback Method
dvisc	0.0002448	Pa×s	511.47	Joback Method
dvisc	0.0001854	Pa×s	550.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.00	K	0.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C774652&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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