Benzene, [(1,1-dimethylethoxy)methyl]-

Other names:	[(1,1-dimethylethoxy)methyl]benzene
	benzyl tert-butyl ether
	ether, benzyl tert-butyl
Inchi:	InChI=1S/C11H16O/c1-11(2,3)12-9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	TZGIRWVSWPFWBP-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CC(C)(C)OCc1ccccc1
Mol. weight [g/mol]:	164.24
CAS:	3459-80-1

Physical Properties

Property code	Value	Unit	Source
gf	51.99	kJ/mol	Joback Method
hf	-174.81	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	43.47	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.002		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	496.95	K	Joback Method
tc	710.44	K	Joback Method
tf	264.80	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.33	J/mol×K	710.44	Joback Method
cpg	345.35	J/mol×K	532.53	Joback Method
cpg	361.23	J/mol×K	568.11	Joback Method
cpg	376.13	J/mol×K	603.69	Joback Method
cpg	390.08	J/mol×K	639.27	Joback Method
cpg	403.13	J/mol×K	674.86	Joback Method

cpg	328.44	J/mol×K	496.95	Joback Method
dvisc	0.0038714	Pa×s	264.80	Joback Method
dvisc	0.0016733	Pa×s	303.49	Joback Method
dvisc	0.0008743	Pa×s	342.18	Joback Method
dvisc	0.0005212	Pa×s	380.88	Joback Method
dvisc	0.0003419	Pa×s	419.57	Joback Method
dvisc	0.0002408	Pa×s	458.26	Joback Method
dvisc	0.0001791	Pa×s	496.95	Joback Method
pvap	0.03	kPa	299.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.02	kPa	296.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.03	kPa	297.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.03	kPa	298.00	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.03	kPa	298.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.02	kPa	295.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.03	kPa	300.30	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers

pvap	0.04	kPa	302.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.04	kPa	303.10	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.04	kPa	303.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.06	kPa	308.00	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.02	kPa	293.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.02	kPa	293.00	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.02	kPa	292.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.01	kPa	290.00	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.01	kPa	288.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers

pvap	0.01	kPa	287.80	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.01	kPa	287.30	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	0.01	kPa	286.20	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	8.93e-03	kPa	284.30	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	7.97e-03	kPa	282.90	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	6.98e-03	kPa	281.30	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	5.77e-03	kPa	279.10	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers
pvap	5.28e-03	kPa	278.10	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers

pvap	5.12e-03	kPa	277.80	Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of Benzyl Alcohol: Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers:	https://www.doi.org/10.1021/je049823k
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=C3459801&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume