

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	m ³ /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/molxK	496.95	Joback Method
dvisc	0.0038714	Paxs	264.80	Joback Method
dvisc	0.0016733	Paxs	303.49	Joback Method
dvisc	0.0008743	Paxs	342.18	Joback Method
dvisc	0.0005212	Paxs	380.88	Joback Method
dvisc	0.0003419	Paxs	419.57	Joback Method
dvisc	0.0002408	Paxs	458.26	Joback Method
dvisc	0.0001791	Paxs	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
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3459801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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