Phenol, 4-(phenylmethoxy)-

Other names:	4-(Benzyloxy)phenol
	4-(phenylmethoxy)phenol
	4-[(phenylmethyl)oxy]phenol
	Agerite
	Agerite alba
	Alba-Dome
	Benoquin
	Benzoquin
	Benzyl hydroquinone
	Benzyl p-hydroxyphenyl ether
	Carmifal
	Depigman
	Dermochinona
	Hydrochinon monobenzylether
	Hydroquinone benzyl ether
	Hydroquinone monobenzyl ether
	Leucodinine
	Monobenzon
	Monobenzyl ether hydroquinone
	Monobenzyl ether of hydroquinone
	Monobenzyl hydroquinone
	NSC 2132
	Phenol, p-(benzyloxy)-
	Pigmex
	Superlite
	Superlite (antioxidant)
	p-(benzyloxy)phenol
	p-Hydroxyphenyl benzyl ether
	para-(Benzyloxy)phenol
Inchi:	InChI=1S/C13H12O2/c14-12-6-8-13(9-7-12)15-10-11-4-2-1-3-5-11/h1-9,14H,10H2
InchiKey:	VYQNWZOUAUKGHI-UHFFFAOYSA-N
Formula:	C13H12O2
SMILES:	Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	200.24

Physical Properties

Property code	Value	Unit	Source

af	0.6443		Cheméo Relay (1.0)
gf	23.78	kJ/mol	Joback Method
hf	-99.51	kJ/mol	Cheméo Relay (1.0)
hfus	24.48	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
log10ws	-2.80		Cheméo Relay (1.0)
logp	2.971		Crippen Method
mcvol	158.250	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	605.40	K	Cheméo Relay (1.0)
tc	867.81	K	Cheméo Relay (1.0)
tf	384.64	K	Cheméo Relay (1.0)
vc	0.571	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.81	J/mol×K	903.38	Joback Method
cpg	415.76	J/mol×K	694.93	Joback Method
cpg	428.94	J/mol×K	736.62	Joback Method
cpg	441.11	J/mol×K	778.31	Joback Method
cpg	452.41	J/mol×K	820.00	Joback Method
cpg	462.93	J/mol×K	861.69	Joback Method
cpg	401.47	J/mol×K	653.24	Joback Method
dvisc	0.0002739	Pa×s	461.42	Joback Method
dvisc	0.0000740	Pa×s	538.15	Joback Method
dvisc	0.0000438	Pa×s	576.51	Joback Method
dvisc	0.0000277	Pa×s	614.88	Joback Method
dvisc	0.0000185	Pa×s	653.24	Joback Method
dvisc	0.0001354	Pa×s	499.79	Joback Method
dvisc	0.0006297	Pa×s	423.06	Joback Method
psub	2.36e-04	kPa	355.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers

psub	3.70e-04	kPa	359.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.16e-04	kPa	349.18	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.16e-04	kPa	349.18	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.40e-04	kPa	351.13	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.46e-04	kPa	351.13	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.46e-04	kPa	351.13	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.89e-04	kPa	353.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.81e-04	kPa	353.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.81e-04	kPa	353.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	

psub	8.70e-05	kPa	347.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	2.33e-04	kPa	355.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	2.33e-04	kPa	355.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	2.94e-04	kPa	357.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	3.05e-04	kPa	357.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	3.05e-04	kPa	357.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	3.90e-04	kPa	359.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.12e-04	kPa	349.18	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	

psub	3.70e-04	kPa	359.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	4.86e-04	kPa	361.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	4.79e-04	kPa	361.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	4.79e-04	kPa	361.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	5.95e-04	kPa	363.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	6.14e-04	kPa	363.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	6.14e-04	kPa	363.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	7.86e-04	kPa	365.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers
psub	7.43e-04	kPa	365.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers

psub	7.43e-04	kPa	365.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	9.67e-04	kPa	367.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	8.70e-05	kPa	347.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	8.60e-05	kPa	347.16	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	9.66e-04	kPa	367.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	9.66e-04	kPa	367.15	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.19e-03	kPa	369.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	
psub	1.24e-03	kPa	369.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers	

psub	1.24e-03	kPa	369.12	Experimental and computational study on the molecular energetics of benzyloxyphenol isomers

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental and computational study on the molecular energetics of benzyloxyphenol isomers:	https://www.doi.org/10.1016/j.jct.2011.06.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103162&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume