

# Acetic acid. (o-benzyloxyphenyl)phenyl-, benzyl ester

Inchi:	InChI=1S/C28H24O3/c29-28(31-21-23-14-6-2-7-15-23)27(24-16-8-3-9-17-24)25-18-10-1
InchiKey:	CSTXHOUFYJFFBP-UHFFFAOYSA-N
Formula:	C28H24O3
SMILES:	O=C(OCc1cccc1)C(c1cccc1)c1cccc1OCc1cccc1
Mol. weight [g/mol]:	408.49
CAS:	116296-22-1

## Physical Properties

Property code	Value	Unit	Source
gf	283.53	kJ/mol	Joback Method
hf	-68.90	kJ/mol	Joback Method
hfus	44.50	kJ/mol	Joback Method
hvap	98.87	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.141		Crippen Method
mcvol	323.650	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
tb	1050.01	K	Joback Method
tc	1312.41	K	Joback Method
tf	602.91	K	Joback Method
vc	1.208	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.17	J/molxK	1050.01	Joback Method
cpg	1075.64	J/molxK	1268.68	Joback Method
cpg	1068.85	J/molxK	1224.94	Joback Method
cpg	1060.95	J/molxK	1181.21	Joback Method
cpg	1051.80	J/molxK	1137.48	Joback Method
cpg	1041.25	J/molxK	1093.74	Joback Method
cpg	1081.46	J/molxK	1312.41	Joback Method
dvisc	0.0000182	Paxs	1050.01	Joback Method
dvisc	0.0000236	Paxs	975.49	Joback Method

dvisc	0.0000319	Paxs	900.98	Joback Method
dvisc	0.0000456	Paxs	826.46	Joback Method
dvisc	0.0000698	Paxs	751.94	Joback Method
dvisc	0.0001175	Paxs	677.43	Joback Method
dvisc	0.0002249	Paxs	602.91	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296221&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296221&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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