Benzaldehyde, 3-(phenylmethoxy)-

Other names:	Benzaldehyde, m-(benzyloxy)-
	m-Benzyloxybenzaldehyde
	3-Benzyloxybenzaldehyde
	Benzyl 3-formylphenyl ether
Inchi:	InChI=1S/C14H12O2/c15-10-13-7-4-8-14(9-13)16-11-12-5-2-1-3-6-12/h1-10H,11H2
InchiKey:	JAICGBJIBWDEIZ-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=Cc1cccc(OCc2ccccc2)c1
Mol. weight [g/mol]:	212.24
CAS:	1700-37-4

Physical Properties

Property code	Value	Unit	Source
gf	77.67	kJ/mol	Joback Method
hf	-88.50	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
log10ws	-3.94		Crippen Method
logp	3.078		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	649.14	K	Joback Method
tc	887.50	K	Joback Method
tf	377.13	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.60	J/mol×K	649.14	Joback Method
cpg	430.38	J/mol×K	688.87	Joback Method
cpg	444.03	J/mol×K	728.59	Joback Method
cpg	456.60	J/mol×K	768.32	Joback Method

cpg	468.14	J/mol×K	808.05	Joback Method
cpg	478.69	J/mol×K	847.77	Joback Method
cpg	488.29	J/mol×K	887.50	Joback Method
dvisc	0.0014593	Pa×s	377.13	Joback Method
dvisc	0.0008357	Pa×s	422.46	Joback Method
dvisc	0.0005332	Pa×s	467.80	Joback Method
dvisc	0.0003683	Pa×s	513.13	Joback Method
dvisc	0.0002702	Pa×s	558.47	Joback Method
dvisc	0.0002076	Pa×s	603.81	Joback Method
dvisc	0.0001655	Pa×s	649.14	Joback Method

Sources

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=C1700374&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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