Benzaldehyde, 3-methoxy-4-(phenylmethoxy)-

Other names:	Benzaldehyde, 4-(benzyloxy)-3-methoxy- 4-(Benzyloxy)-3-methoxybenzaldehyde Benzylvanillin O-Benzylvanillin 4-O-Benzylvanillin 3-Methoxy-4-(benzyloxy)benzaldehyde Vanillin benzyl ether Benzaldehyde, 4-benzyloxy-5-methoxy- 3-Methoxy-4-(phenylmethoxy)benzaldehyde NSC 208757 NSC 22599 NSC 44876
Inchi:	InChI=1S/C15H14O3/c1-17-15-9-13(10-16)7-8-14(15)18-11-12-5-3-2-4-6-12/h2-10H,11H
InchiKey:	JSHLOPGSDZTEGQ-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	COc1cc(C=O)ccc1OCc1ccccc1
Mol. weight [g/mol]:	242.27
CAS:	2426-87-1

Physical Properties

Property code	Value	Unit	Source
gf	-28.54	kJ/mol	Joback Method
hf	-252.83	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.087		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	699.42	K	Joback Method
tc	930.48	K	Joback Method
tf	423.15	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.93	J/mol×K	699.42	Joback Method
cpg	553.77	J/mol×K	891.97	Joback Method
cpg	543.29	J/mol×K	853.46	Joback Method
cpg	531.79	J/mol×K	814.95	Joback Method
cpg	519.24	J/mol×K	776.44	Joback Method
cpg	505.63	J/mol×K	737.93	Joback Method
cpg	563.24	J/mol×K	930.48	Joback Method
dvisc	0.0001178	Pa×s	699.42	Joback Method
dvisc	0.0001460	Pa×s	653.38	Joback Method
dvisc	0.0001868	Pa×s	607.33	Joback Method
dvisc	0.0002488	Pa×s	561.29	Joback Method
dvisc	0.0003489	Pa×s	515.24	Joback Method
dvisc	0.0005229	Pa×s	469.19	Joback Method
dvisc	0.0008558	Pa×s	423.15	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2426871&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume