Benzaldehyde, 3-(4-methoxyphenoxy)-

Other names: 3-(4-Methoxyphenoxy)benzaldehyde
Inchi: InChI=1S/C14H12O3/c1-16-12-5-7-13(8-6-12)17-14-4-2-3-11(9-14)10-15/h2-10H,1H3
InchiKey: WLFDEVVCXPTAQA-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: COc1ccc(Oc2cccc(C=O)c2)cc1
Mol. weight [g/mol]: 228.24
CAS: 62373-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-36.96	kJ/mol	Joback Method
hf	-232.19	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.300		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	676.54	K	Joback Method
tc	912.18	K	Joback Method
tf	411.88	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.53	J/mol×K	676.54	Joback Method
cpg	453.74	J/mol×K	715.81	Joback Method
cpg	466.90	J/mol×K	755.09	Joback Method
cpg	479.02	J/mol×K	794.36	Joback Method
cpg	490.13	J/mol×K	833.63	Joback Method
cpg	500.23	J/mol×K	872.90	Joback Method
cpg	509.35	J/mol×K	912.18	Joback Method
dvisc	0.0008979	Pa×s	411.88	Joback Method

dvisc	0.0005575	Pa×s	455.99	Joback Method
dvisc	0.0003764	Pa×s	500.10	Joback Method
dvisc	0.0002709	Pa×s	544.21	Joback Method
dvisc	0.0002048	Pa×s	588.32	Joback Method
dvisc	0.0001610	Pa×s	632.43	Joback Method
dvisc	0.0001306	Pa×s	676.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	0.05	NIST Webbook

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=C62373802&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume