Benzaldehyde, 3,4,5-trimethoxy-

Other names:	3,4,5-Trimethoxybenzaldehyde
Inchi:	InChI=1S/C10H12O4/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-6H,1-3H3
InchiKey:	OPHQOIGEOHXOGX-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cc(C=O)cc(OC)c1OC
Mol. weight [g/mol]:	196.20
CAS:	86-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-297.68	kJ/mol	Joback Method
hf	-529.85	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.525		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1608.00		NIST Webbook
ripol	2539.00		NIST Webbook
tb	585.74	K	Joback Method
tc	792.23	K	Joback Method
tf	375.13	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.43	J/mol×K	585.74	Joback Method
cpg	402.61	J/mol×K	757.82	Joback Method
cpg	392.68	J/mol×K	723.40	Joback Method
cpg	382.17	J/mol×K	688.99	Joback Method

cpg	371.11	J/mol×K	654.57	Joback Method
cpg	359.52	J/mol×K	620.16	Joback Method
cpg	411.94	J/mol×K	792.23	Joback Method
dvisc	0.0001477	Pa×s	585.74	Joback Method
dvisc	0.0001775	Pa×s	550.64	Joback Method
dvisc	0.0002187	Pa×s	515.54	Joback Method
dvisc	0.0002780	Pa×s	480.44	Joback Method
dvisc	0.0003668	Pa×s	445.33	Joback Method
dvisc	0.0005076	Pa×s	410.23	Joback Method
dvisc	0.0007464	Pa×s	375.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86817&Units=SI
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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