

Benzaldehyde, 2,3,4-trimethoxy-

Other names:	2,3,4-Trimethoxybenzaldehyde
Inchi:	InChI=1S/C10H12O4/c1-12-8-5-4-7(6-11)9(13-2)10(8)14-3/h4-6H,1-3H3
InchiKey:	UCTUXUGXIFRVGX-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	<chem>COc1ccc(C=O)c(OC)c1OC</chem>
Mol. weight [g/mol]:	196.20
CAS:	2103-57-3

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
tb	585.74	K	Joback Method
tc	792.23	K	Joback Method
tf	375.13	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.43	J/molxK	585.74	Joback Method
cpg	359.52	J/molxK	620.16	Joback Method
cpg	371.11	J/molxK	654.57	Joback Method
cpg	382.17	J/molxK	688.99	Joback Method
cpg	392.68	J/molxK	723.40	Joback Method
cpg	402.61	J/molxK	757.82	Joback Method
cpg	411.94	J/molxK	792.23	Joback Method
dvisc	0.0007464	Paxs	375.13	Joback Method

dvisc	0.0005076	Paxs	410.23	Joback Method
dvisc	0.0003668	Paxs	445.33	Joback Method
dvisc	0.0002780	Paxs	480.44	Joback Method
dvisc	0.0002187	Paxs	515.54	Joback Method
dvisc	0.0001775	Paxs	550.64	Joback Method
dvisc	0.0001477	Paxs	585.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2103573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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