

Benzaldehyde, 2,4,5-trimethoxy-

Other names:	2,4,5-Trimethoxybenzaldehyde Asaronaldehyde Asaraldehyde 3,4,6-Trimethoxybenzaldehyde Azarylaldehyde Gazarin NCI-C61632 NSC 89299
Inchi:	InChI=1S/C10H12O4/c1-12-8-5-10(14-3)9(13-2)4-7(8)6-11/h4-6H,1-3H3
InchiKey:	IAJBQAYHSQIQRE-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	<chem>COc1cc(OC)c(OC)cc1C=O</chem>
Mol. weight [g/mol]:	196.20
CAS:	4460-86-0

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	1620.00		NIST Webbook
ripol	2233.00		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	359.52	J/mol×K	620.16	Joback Method
cpg	371.11	J/mol×K	654.57	Joback Method
cpg	382.17	J/mol×K	688.99	Joback Method
cpg	392.68	J/mol×K	723.40	Joback Method
cpg	402.61	J/mol×K	757.82	Joback Method
cpg	411.94	J/mol×K	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

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=C4460860&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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