Benzaldehyde, 2,5-dimethoxy-

Other names: 2,5-Dimethoxybenzaldehyde
Inchi: InChI=1S/C9H10O3/c1-11-8-3-4-9(12-2)7(5-8)6-10/h3-6H,1-2H3
InchiKey: AFUKNJHPZAVHGQ-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: COc1ccc(OC)c(C=O)c1
Mol. weight [g/mol]: 166.18

Physical Properties

Property code	Value	Unit	Source
hf	-352.20	kJ/mol	Cheméo Relay (1.0)
hfus	16.99	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-2.32		Aqueous Solubility Prediction Method
logp	1.516		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
rinpol	1471.20		NIST Webbook
rinpol	1471.20		NIST Webbook
ripol	2278.00		NIST Webbook
tb	552.83	K	Cheméo Relay (1.0)
tf	319.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.82	J/mol×K	535.46	Joback Method
cpg	291.21	J/mol×K	570.62	Joback Method
cpg	302.11	J/mol×K	605.77	Joback Method
cpg	312.49	J/mol×K	640.93	Joback Method
cpg	322.35	J/mol×K	676.09	Joback Method
cpg	331.68	J/mol×K	711.24	Joback Method
cpg	340.46	J/mol×K	746.40	Joback Method
dvisc	0.0011750	Pa×s	329.11	Joback Method

dvisc	0.0007578	Pa×s	363.50	Joback Method
dvisc	0.0005273	Pa×s	397.89	Joback Method
dvisc	0.0003887	Pa×s	432.29	Joback Method
dvisc	0.0002996	Pa×s	466.68	Joback Method
dvisc	0.0002394	Pa×s	501.07	Joback Method
dvisc	0.0001969	Pa×s	535.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93027&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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