

3,5-Dimethoxybenzaldehyde

Other names:	Benzaldehyde, 3,5-dimethoxy- Benzaldehyde, 3,5-dimethoxy
Inchi:	InChI=1S/C9H10O3/c1-11-8-3-7(6-10)4-9(5-8)12-2/h3-6H,1-2H3
InchiKey:	VFZRZRDOXPRTSC-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cc(C=O)cc(OC)c1
Mol. weight [g/mol]:	166.17
CAS:	7311-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-191.47	kJ/mol	Joback Method
hf	-365.52	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.516		Crippen Method
mvol	127.220	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	535.46	K	Joback Method
tc	746.40	K	Joback Method
tf	329.11	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.82	J/molxK	535.46	Joback Method
cpg	331.68	J/molxK	711.24	Joback Method
cpg	322.35	J/molxK	676.09	Joback Method
cpg	312.49	J/molxK	640.93	Joback Method
cpg	302.11	J/molxK	605.77	Joback Method
cpg	291.21	J/molxK	570.62	Joback Method
cpg	340.46	J/molxK	746.40	Joback Method

dvisc	0.0001969	Paxs	535.46	Joback Method
dvisc	0.0002394	Paxs	501.07	Joback Method
dvisc	0.0002996	Paxs	466.68	Joback Method
dvisc	0.0003887	Paxs	432.29	Joback Method
dvisc	0.0005273	Paxs	397.89	Joback Method
dvisc	0.0007578	Paxs	363.50	Joback Method
dvisc	0.0011750	Paxs	329.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	2.10	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7311344&Units=SI

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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