

2,3-Dimethoxybenzoic acid

Other names:	Benzoic acid, 2,3-dimethoxy- o-Veratric acid
Inchi:	InChI=1S/C9H10O4/c1-12-7-5-3-4-6(9(10)11)8(7)13-2/h3-5H,1-2H3,(H,10,11)
InchiKey:	FODBVCSYJKNBLO-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COc1cccc(C(=O)O)c1OC
Mol. weight [g/mol]:	182.17
CAS:	1521-38-6

Physical Properties

Property code	Value	Unit	Source
chs	-4283.80 ± 0.80	kJ/mol	NIST Webbook
gf	-357.69	kJ/mol	Joback Method
hf	-544.75	kJ/mol	Joback Method
hfs	-687.00 ± 1.40	kJ/mol	NIST Webbook
hfus	20.39	kJ/mol	Joback Method
hsub	116.60 ± 0.30	kJ/mol	NIST Webbook
hsub	116.60 ± 0.30	kJ/mol	NIST Webbook
hvap	67.47	kJ/mol	Joback Method
log10ws	-2.14		Aqueous Solubility Prediction Method
logp	1.402		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	632.85	K	Joback Method
tc	834.15	K	Joback Method
tf	397.86	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	376.13	J/molxK	834.15	Joback Method
cpg	368.87	J/molxK	800.60	Joback Method
cpg	361.07	J/molxK	767.05	Joback Method
cpg	352.73	J/molxK	733.50	Joback Method
cpg	343.86	J/molxK	699.95	Joback Method
cpg	334.47	J/molxK	666.40	Joback Method
cpg	324.57	J/molxK	632.85	Joback Method
dvisc	0.0012398	Paxs	397.86	Joback Method
dvisc	0.0000571	Paxs	632.85	Joback Method
dvisc	0.0000805	Paxs	593.68	Joback Method
dvisc	0.0001191	Paxs	554.52	Joback Method
dvisc	0.0001872	Paxs	515.36	Joback Method
dvisc	0.0003170	Paxs	476.19	Joback Method
dvisc	0.0005897	Paxs	437.03	Joback Method
hsubt	115.10 ± 0.30	kJ/mol	346.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1521386&Units=SI>

Crippen Method:

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

Joback Method:

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

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
h vap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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