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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	324.57	J/mol×K	632.85	Joback Method
cpg	334.47	J/mol×K	666.40	Joback Method
cpg	343.86	J/mol×K	699.95	Joback Method
cpg	352.73	J/mol×K	733.50	Joback Method
cpg	361.07	J/mol×K	767.05	Joback Method
cpg	368.87	J/mol×K	800.60	Joback Method
cpg	376.13	J/mol×K	834.15	Joback Method
dvisc	0.0012398	Pa×s	397.86	Joback Method
dvisc	0.0005897	Pa×s	437.03	Joback Method
dvisc	0.0003170	Pa×s	476.19	Joback Method
dvisc	0.0001872	Pa×s	515.36	Joback Method
dvisc	0.0001191	Pa×s	554.52	Joback Method
dvisc	0.0000805	Pa×s	593.68	Joback Method
dvisc	0.0000571	Pa×s	632.85	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/ci990307l
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
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
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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