Benzoic acid, 2,6-dimethoxy-

Other names: 2,6-Dimethoxybenzoic acid
Inchi: InChI=1S/C9H10O4/c1-12-6-4-3-5-7(13-2)8(6)9(10)11/h3-5H,1-2H3,(H,10,11)
InchiKey: MBIZFBDREVRUHY-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: COc1cccc(OC)c1C(=O)O
Mol. weight [g/mol]: 182.17
CAS: 1466-76-8

Physical Properties

Property code	Value	Unit	Source
chs	-4276.90 ± 0.80	kJ/mol	NIST Webbook
gf	-357.69	kJ/mol	Joback Method
hf	-544.75	kJ/mol	Joback Method
hfs	-693.80 ± 1.40	kJ/mol	NIST Webbook
hfus	20.39	kJ/mol	Joback Method
hsub	121.70 ± 0.40	kJ/mol	NIST Webbook
hsub	121.70 ± 0.40	kJ/mol	NIST Webbook
hvap	67.47	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.402		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1460.00		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	376.13	J/mol×K	834.15	Joback Method
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
dvisc	0.0000571	Pa×s	632.85	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
hsubt	118.40 ± 0.40	kJ/mol	356.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1466768&Units=SI
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

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