2,4,6-Trimethoxybenzoic acid

Other names: Benzoic acid, 2,4,6-trimethoxy-
Inchi: InChI=1S/C10H12O5/c1-13-6-4-7(14-2)9(10(11)12)8(5-6)15-3/h4-5H,1-3H3,(H,11,12)
InchiKey: JATAKEDDMQNPOQ-UHFFFAOYSA-N
Formula: C10H12O5
SMILES: COc1cc(OC)c(C(=O)O)c(OC)c1
Mol. weight [g/mol]: 212.20
CAS: 570-02-5

Physical Properties

Property code	Value	Unit	Source
gf	-463.90	kJ/mol	Joback Method
hf	-709.08	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.411		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	683.13	K	Joback Method
tc	881.29	K	Joback Method
tf	443.88	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.28	J/mol×K	683.13	Joback Method
cpg	405.78	J/mol×K	716.16	Joback Method
cpg	415.73	J/mol×K	749.18	Joback Method
cpg	425.10	J/mol×K	782.21	Joback Method
cpg	433.87	J/mol×K	815.24	Joback Method
cpg	442.01	J/mol×K	848.26	Joback Method

cpg	449.51	J/mol×K	881.29	Joback Method
dvisc	0.0005426	Pa×s	443.88	Joback Method
dvisc	0.0002852	Pa×s	483.75	Joback Method
dvisc	0.0001653	Pa×s	523.63	Joback Method
dvisc	0.0001035	Pa×s	563.50	Joback Method
dvisc	0.0000690	Pa×s	603.38	Joback Method
dvisc	0.0000483	Pa×s	643.25	Joback Method
dvisc	0.0000353	Pa×s	683.13	Joback Method

Sources

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=C570025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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