Benzoic acid, 2,4-dimethyl-, methyl ester

Other names: Methyl 2,4-dimethylbenzoate
2,4-(CH3)2-C6H3-COOCH3
Inchi: InChI=1S/C10H12O2/c1-7-4-5-9(8(2)6-7)10(11)12-3/h4-6H,1-3H3
InchiKey: QQCLNRPRQRDMCK-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: COC(=O)c1ccc(C)cc1C
Mol. weight [g/mol]: 164.20
CAS: 23617-71-2

Physical Properties

Property code	Value	Unit	Source
affp	868.20	kJ/mol	NIST Webbook
basg	837.20	kJ/mol	NIST Webbook
gf	-107.45	kJ/mol	Joback Method
hf	-280.94	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.090		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	220.82		NIST Webbook
ripol	1821.00		NIST Webbook
tb	505.70	K	NIST Webbook
tc	756.04	K	Joback Method
tf	326.08	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.97	J/mol×K	541.13	Joback Method
cpg	358.27	J/mol×K	720.22	Joback Method

cpg	347.89	J/mol×K	684.40	Joback Method
cpg	336.88	J/mol×K	648.58	Joback Method
cpg	325.22	J/mol×K	612.77	Joback Method
cpg	312.92	J/mol×K	576.95	Joback Method
cpg	368.03	J/mol×K	756.04	Joback Method
dvisc	0.0002040	Pa×s	541.13	Joback Method
dvisc	0.0002500	Pa×s	505.29	Joback Method
dvisc	0.0003161	Pa×s	469.45	Joback Method
dvisc	0.0004153	Pa×s	433.61	Joback Method
dvisc	0.0005733	Pa×s	397.76	Joback Method
dvisc	0.0008436	Pa×s	361.92	Joback Method
dvisc	0.0013513	Pa×s	326.08	Joback Method

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=C23617712&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume