

Benzoic acid, 2,6-dimethyl-, methyl ester

Other names:	Methyl 2,6-dimethylbenzoate 2,6-(CH ₃) ₂ -C ₆ H ₃ -COOCH ₃
Inchi:	InChI=1S/C10H12O2/c1-7-5-4-6-8(2)9(7)10(11)12-3/h4-6H,1-3H3
InchiKey:	XJMULMWDHLJUKP-UHFFFAOYSA-N
Formula:	C ₁₀ H ₁₂ O ₂
SMILES:	COC(=O)c1c(C)ccc1C
Mol. weight [g/mol]:	164.20
CAS:	14920-81-1

Physical Properties

Property code	Value	Unit	Source
affp	855.30	kJ/mol	NIST Webbook
basg	824.30	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	1239.00		NIST Webbook
rinpol	210.24		NIST Webbook
rinpol	210.24		NIST Webbook
tb	541.13	K	Joback Method
tc	756.04	K	Joback Method
tf	326.08	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.97	J/mol×K	541.13	Joback Method
cpg	312.92	J/mol×K	576.95	Joback Method

cpg	325.22	J/molxK	612.77	Joback Method
cpg	336.88	J/molxK	648.58	Joback Method
cpg	347.89	J/molxK	684.40	Joback Method
cpg	358.27	J/molxK	720.22	Joback Method
cpg	368.03	J/molxK	756.04	Joback Method
dvisc	0.0013513	Paxs	326.08	Joback Method
dvisc	0.0008436	Paxs	361.92	Joback Method
dvisc	0.0005733	Paxs	397.76	Joback Method
dvisc	0.0004153	Paxs	433.61	Joback Method
dvisc	0.0003161	Paxs	469.45	Joback Method
dvisc	0.0002500	Paxs	505.29	Joback Method
dvisc	0.0002040	Paxs	541.13	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=C14920811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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