

Methyl 3-methoxy-4-methylbenzoate

Other names:	Benzoic acid, 4-methyl-3-methoxy, methyl ester Benzoic acid, 3-methoxy-4-methyl-, methyl ester 3-methoxy-4-methylbenzoesauremethylester
Inchi:	InChI=1S/C10H12O3/c1-7-4-5-8(10(11)13-3)6-9(7)12-2/h4-6H,1-3H3
InchiKey:	LLEXCSBUSVRBCA-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COC(=O)c1ccc(C)c(OC)c1
Mol. weight [g/mol]:	180.20
CAS:	3556-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-212.45	kJ/mol	Joback Method
hf	-413.16	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.790		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	563.55	K	Joback Method
tc	776.08	K	Joback Method
tf	348.31	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.48	J/mol×K	563.55	Joback Method
cpg	336.25	J/mol×K	598.97	Joback Method
cpg	348.42	J/mol×K	634.39	Joback Method
cpg	359.98	J/mol×K	669.82	Joback Method
cpg	370.92	J/mol×K	705.24	Joback Method
cpg	381.23	J/mol×K	740.66	Joback Method

cpg	390.91	J/mol×K	776.08	Joback Method
dvisc	0.0010565	Pa×s	348.31	Joback Method
dvisc	0.0006746	Pa×s	384.18	Joback Method
dvisc	0.0004650	Pa×s	420.06	Joback Method
dvisc	0.0003399	Pa×s	455.93	Joback Method
dvisc	0.0002601	Pa×s	491.80	Joback Method
dvisc	0.0002064	Pa×s	527.68	Joback Method
dvisc	0.0001686	Pa×s	563.55	Joback Method

Sources

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=C3556830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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