Methyl 4-methoxy-3-methylbenzoate

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

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
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
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	381.23	J/mol×K	740.66	Joback Method
cpg	370.92	J/mol×K	705.24	Joback Method
cpg	359.98	J/mol×K	669.82	Joback Method
cpg	348.42	J/mol×K	634.39	Joback Method
cpg	336.25	J/mol×K	598.97	Joback Method
cpg	390.91	J/mol×K	776.08	Joback Method

dvisc	0.0001686	Pa×s	563.55	Joback Method
dvisc	0.0002064	Pa×s	527.68	Joback Method
dvisc	0.0002601	Pa×s	491.80	Joback Method
dvisc	0.0003399	Pa×s	455.93	Joback Method
dvisc	0.0004650	Pa×s	420.06	Joback Method
dvisc	0.0006746	Pa×s	384.18	Joback Method
dvisc	0.0010565	Pa×s	348.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378753&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

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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