Benzoic acid, 4-(acetyloxy)-3-methoxy-, methyl ester

Other names: Methyl 3-methoxy-4-acetoxybenzoate
Methyl 4-(acetyloxy)-3-methoxybenzoate
Inchi: InChI=1S/C11H12O5/c1-7(12)16-9-5-4-8(11(13)15-3)6-10(9)14-2/h4-6H,1-3H3
InchiKey: BHQRCCUOSHDJQC-UHFFFAOYSA-N
Formula: C11H12O5
SMILES: COC(=O)c1ccc(OC(C)=O)c(OC)c1
Mol. weight [g/mol]: 224.21
CAS: 35400-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-437.95	kJ/mol	Joback Method
hf	-678.60	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.407		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1663.20		NIST Webbook
rinpol	1663.20		NIST Webbook
tb	662.72	K	Joback Method
tc	876.45	K	Joback Method
tf	431.74	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.14	J/mol×K	662.72	Joback Method
cpg	464.41	J/mol×K	840.83	Joback Method
cpg	455.09	J/mol×K	805.21	Joback Method
cpg	444.98	J/mol×K	769.58	Joback Method
cpg	434.10	J/mol×K	733.96	Joback Method

cpg	422.48	J/mol×K	698.34	Joback Method
cpg	472.91	J/mol×K	876.45	Joback Method
dvisc	0.0001295	Pa×s	662.72	Joback Method
dvisc	0.0001580	Pa×s	624.22	Joback Method
dvisc	0.0001978	Pa×s	585.73	Joback Method
dvisc	0.0002557	Pa×s	547.23	Joback Method
dvisc	0.0003435	Pa×s	508.73	Joback Method
dvisc	0.0004844	Pa×s	470.24	Joback Method
dvisc	0.0007263	Pa×s	431.74	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35400192&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

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