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

Other names:	Benzoic acid, m-hydroxy-, methyl ester, acetate
	Methyl m-acetoxybenzoate
	3-Acetoxybenzoesaeure-methylester
	3-Acetoxybenzoic acid, methyl ester
	Methyl 3-acetyloxybenzoate
Inchi:	InChI=1S/C10H10O4/c1-7(11)14-9-5-3-4-8(6-9)10(12)13-2/h3-6H,1-2H3
InchiKey:	QVHJKRQXHIMCTL-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COC(=O)c1cccc(OC(C)=O)c1
Mol. weight [g/mol]:	194.18
CAS:	24781-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-331.74	kJ/mol	Joback Method
hf	-514.27	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.398		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1490.00		NIST Webbook
tb	612.44	K	Joback Method
tc	831.50	K	Joback Method
tf	385.72	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.80	J/mol×K	612.44	Joback Method
cpg	391.31	J/mol×K	794.99	Joback Method
cpg	382.23	J/mol×K	758.48	Joback Method

cpg	372.43	J/mol×K	721.97	Joback Method
cpg	361.93	J/mol×K	685.46	Joback Method
cpg	350.71	J/mol×K	648.95	Joback Method
cpg	399.66	J/mol×K	831.50	Joback Method
dvisc	0.0001824	Pa×s	612.44	Joback Method
dvisc	0.0002254	Pa×s	574.65	Joback Method
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0003788	Pa×s	499.08	Joback Method
dvisc	0.0005235	Pa×s	461.29	Joback Method
dvisc	0.0007664	Pa×s	423.51	Joback Method
dvisc	0.0012091	Pa×s	385.72	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=C24781235&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume