Benzoic acid, 4-acetyl-, methyl ester

Other names: 4-Acetylbenzoic acid, methyl
Inchi: InChI=1S/C10H10O3/c1-7(11)8-3-5-9(6-4-8)10(12)13-2/h3-6H,1-2H3
InchiKey: QNTSFZXGLAHYLC-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: COC(=O)c1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 178.18
CAS: 3609-53-8

Physical Properties

Property code	Value	Unit	Source
ea	0.96 ± 0.09	eV	NIST Webbook
ea	0.94 ± 0.09	eV	NIST Webbook
gf	-226.74	kJ/mol	Joback Method
hf	-382.05	kJ/mol	Joback Method
hfus	19.69	kJ/mol	Joback Method
hvap	56.69	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.676		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	590.02	K	Joback Method
tc	811.87	K	Joback Method
tf	363.49	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.55	J/mol×K	590.02	Joback Method
cpg	368.72	J/mol×K	774.89	Joback Method
cpg	359.51	J/mol×K	737.92	Joback Method
cpg	349.60	J/mol×K	700.94	Joback Method

cpg	338.98	J/mol×K	663.97	Joback Method
cpg	327.63	J/mol×K	626.99	Joback Method
cpg	377.23	J/mol×K	811.87	Joback Method
dvisc	0.0002262	Pa×s	590.02	Joback Method
dvisc	0.0002803	Pa×s	552.26	Joback Method
dvisc	0.0003583	Pa×s	514.51	Joback Method
dvisc	0.0004763	Pa×s	476.75	Joback Method
dvisc	0.0006648	Pa×s	439.00	Joback Method
dvisc	0.0009880	Pa×s	401.25	Joback Method
dvisc	0.0015944	Pa×s	363.49	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3609538&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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