4-Acetoxyacetophenone

Other names:	4-Acetylphenyl acetate
	p-Acetoxyacetophenone
	Ethanone, 1-[4-(acetyloxy)phenyl]-
	4-CH3COO-C6H4-COCH3
	p-acetylphenyl acetate
Inchi:	InChI=1S/C10H10O3/c1-7(11)9-3-5-10(6-4-9)13-8(2)12/h3-6H,1-2H3
InchiKey:	SMIOEQSLJNNKQF-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	178.18
CAS:	13031-43-1

Physical Properties

Property code	Value	Unit	Source
affp	853.20	kJ/mol	NIST Webbook
basg	821.30	kJ/mol	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	-2.45		Crippen Method
logp	1.814		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
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	327.63	J/mol×K	626.99	Joback Method

cpg	338.98	J/mol×K	663.97	Joback Method
cpg	349.60	J/mol×K	700.94	Joback Method
cpg	359.51	J/mol×K	737.92	Joback Method
cpg	368.72	J/mol×K	774.89	Joback Method
cpg	377.23	J/mol×K	811.87	Joback Method
dvisc	0.0015944	Pa×s	363.49	Joback Method
dvisc	0.0009880	Pa×s	401.25	Joback Method
dvisc	0.0006648	Pa×s	439.00	Joback Method
dvisc	0.0004763	Pa×s	476.75	Joback Method
dvisc	0.0003583	Pa×s	514.51	Joback Method
dvisc	0.0002803	Pa×s	552.26	Joback Method
dvisc	0.0002262	Pa×s	590.02	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=C13031431&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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