4-(p-Acetoxyphenyl)-2-butanone

Other names:	p-(3-Oxobutyl)phenyl acetate
	2-Butanone, 4-[4-(acetyloxy)phenyl]-
	para-(2-Acetylethyl)phenyl acetate
	Q-Lure
	Acetate of 4-(hydroxyphenyl)-2-butanone
	Cue-lure
	ENT-32833
	Pherocon QFF
	2-Butanone, 4-(p-hydroxyphenyl)-, acetate
	4-(p-Hydroxyphenyl)-2-butanone, acetate
	4-(4-Acetoxyphenyl)-2-butanone
	NSC 39438
	4-(3-oxobutyl)phenyl acetate
Inchi:	InChI=1S/C12H14O3/c1-9(13)3-4-11-5-7-12(8-6-11)15-10(2)14/h5-8H,3-4H2,1-2H3
InchiKey:	UMIKWXDGXDJQJK-UHFFFAOYSA-N
Formula:	C12H14O3
SMILES:	CC(=O)CCc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]:	206.24
CAS:	3572-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-209.90	kJ/mol	Joback Method
hf	-423.33	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.133		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	635.78	K	Joback Method
tc	849.97	K	Joback Method
tf	386.03	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.51	J/mol×K	635.78	Joback Method
cpg	425.11	J/mol×K	671.48	Joback Method
cpg	437.88	J/mol×K	707.18	Joback Method
cpg	449.83	J/mol×K	742.87	Joback Method
cpg	460.99	J/mol×K	778.57	Joback Method
cpg	471.37	J/mol×K	814.27	Joback Method
cpg	480.98	J/mol×K	849.97	Joback Method
dvisc	0.0015002	Pa×s	386.03	Joback Method
dvisc	0.0008976	Pa×s	427.66	Joback Method
dvisc	0.0005883	Pa×s	469.28	Joback Method
dvisc	0.0004131	Pa×s	510.90	Joback Method
dvisc	0.0003059	Pa×s	552.53	Joback Method
dvisc	0.0002363	Pa×s	594.15	Joback Method
dvisc	0.0001888	Pa×s	635.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	0.03	NIST Webbook

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=C3572063&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume