Ethanone, 2-(acetyloxy)-1,2-diphenyl-

Other names: Benzoin, acetate
O-Acetylbenzoin
Inchi: InChI=1S/C16H14O3/c1-12(17)19-16(14-10-6-3-7-11-14)15(18)13-8-4-2-5-9-13/h2-11,16
InchiKey: QRWAIZJYJNLOPG-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: CC(=O)OC(C(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 254.28
CAS: 574-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-56.62	kJ/mol	Joback Method
hf	-263.17	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.174		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	748.56	K	Joback Method
tc	991.46	K	Joback Method
tf	430.01	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.59	J/mol×K	748.56	Joback Method
cpg	549.02	J/mol×K	789.04	Joback Method
cpg	562.17	J/mol×K	829.53	Joback Method
cpg	574.09	J/mol×K	870.01	Joback Method
cpg	584.84	J/mol×K	910.50	Joback Method
cpg	594.50	J/mol×K	950.98	Joback Method
cpg	603.12	J/mol×K	991.46	Joback Method

dvisc	0.0013883	Pa×s	430.01	Joback Method
dvisc	0.0007261	Pa×s	483.10	Joback Method
dvisc	0.0004317	Pa×s	536.19	Joback Method
dvisc	0.0002819	Pa×s	589.29	Joback Method
dvisc	0.0001976	Pa×s	642.38	Joback Method
dvisc	0.0001461	Pa×s	695.47	Joback Method
dvisc	0.0001128	Pa×s	748.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C574061&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume