3-(2-Acetoxy-2-propyl)indene

Inchi: InChI=1S/C14H16O2/c1-10(15)16-14(2,3)13-9-8-11-6-4-5-7-12(11)13/h4-7,9H,8H2,1-3H
InchiKey: AQCVGMNRJOFKDO-UHFFFAOYSA-N
Formula: C14H16O2
SMILES: CC(=O)OC(C)(C)C1=CCc2ccccc21
Mol. weight [g/mol]: 216.28
CAS: 42447-90-5

Physical Properties

Property code	Value	Unit	Source
gf	27.49	kJ/mol	Joback Method
hf	-221.33	kJ/mol	Joback Method
hfus	18.94	kJ/mol	Joback Method
hvap	58.73	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.968		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	639.99	K	Joback Method
tc	869.91	K	Joback Method
tf	396.52	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.71	J/mol×K	639.99	Joback Method
cpg	473.27	J/mol×K	678.31	Joback Method
cpg	487.69	J/mol×K	716.63	Joback Method
cpg	501.06	J/mol×K	754.95	Joback Method
cpg	513.47	J/mol×K	793.27	Joback Method
cpg	525.01	J/mol×K	831.59	Joback Method
cpg	535.77	J/mol×K	869.91	Joback Method
dvisc	0.0016082	Pa×s	396.52	Joback Method
dvisc	0.0010541	Pa×s	437.10	Joback Method

dvisc	0.0007423	Pa×s	477.68	Joback Method
dvisc	0.0005522	Pa×s	518.25	Joback Method
dvisc	0.0004289	Pa×s	558.83	Joback Method
dvisc	0.0003446	Pa×s	599.41	Joback Method
dvisc	0.0002848	Pa×s	639.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42447905&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