

1-(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/h4-9,13H,1-3H3
InchiKey:	OPRJCZZHDXMQBA-UHFFFAOYSA-N
Formula:	C14H16O2
SMILES:	CC(=O)OC(C)(C)C1C=Cc2ccccc21
Mol. weight [g/mol]:	216.28
CAS:	42271-88-5

Physical Properties

Property code	Value	Unit	Source
gf	29.41	kJ/mol	Joback Method
hf	-230.20	kJ/mol	Joback Method
hfus	20.40	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.139		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	630.34	K	Joback Method
tc	859.41	K	Joback Method
tf	379.76	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.59	J/molxK	630.34	Joback Method
cpg	476.92	J/molxK	668.52	Joback Method
cpg	492.04	J/molxK	706.70	Joback Method
cpg	506.04	J/molxK	744.87	Joback Method
cpg	519.00	J/molxK	783.05	Joback Method
cpg	531.03	J/molxK	821.23	Joback Method
cpg	542.20	J/molxK	859.41	Joback Method
dvisc	0.0018107	Paxs	379.76	Joback Method
dvisc	0.0011903	Paxs	421.52	Joback Method

dvisc	0.0008439	Paxs	463.29	Joback Method
dvisc	0.0006334	Paxs	505.05	Joback Method
dvisc	0.0004966	Paxs	546.81	Joback Method
dvisc	0.0004031	Paxs	588.58	Joback Method
dvisc	0.0003364	Paxs	630.34	Joback Method

Sources

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=C42271885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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