5-Phenyl-2,4-pentadienyl acetate

Inchi: InChI=1S/C13H14O2/c1-12(14)15-11-7-3-6-10-13-8-4-2-5-9-13/h2-10H,11H2,1H3/b7-3+
InchiKey: HSOAIIIEPRQXKY-ASVGJQBISA-N
Formula: C13H14O2
SMILES: CC(=O)OCC=CC=Cc1ccccc1
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	97.51	kJ/mol	Joback Method
hf	-85.48	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	55.88	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.819		Crippen Method
mcvol	169.110	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	608.13	K	Joback Method
tc	828.54	K	Joback Method
tf	324.69	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.59	J/mol×K	608.13	Joback Method
cpg	417.33	J/mol×K	644.87	Joback Method
cpg	431.09	J/mol×K	681.60	Joback Method
cpg	443.92	J/mol×K	718.34	Joback Method
cpg	455.88	J/mol×K	755.07	Joback Method
cpg	467.03	J/mol×K	791.81	Joback Method
cpg	477.44	J/mol×K	828.54	Joback Method
dvisc	0.0018445	Pa×s	324.69	Joback Method

dvisc	0.0008811	Pa×s	371.93	Joback Method
dvisc	0.0004971	Pa×s	419.17	Joback Method
dvisc	0.0003150	Pa×s	466.41	Joback Method
dvisc	0.0002170	Pa×s	513.65	Joback Method
dvisc	0.0001592	Pa×s	560.89	Joback Method
dvisc	0.0001226	Pa×s	608.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R181709&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume