Acetic acid, phenyl-, 3-hexenyl ester

Other names:	3-Hexenyl phenylacetate
Inchi:	InChI=1S/C14H18O2/c1-2-3-4-8-11-16-14(15)12-13-9-6-5-7-10-13/h3-7,9-10H,2,8,11-12
InchiKey:	FJKFIIYSBXHBCT-ONEGZZNKSA-N
Formula:	C14H18O2
SMILES:	CCC=CCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	25.71	kJ/mol	Joback Method
hf	-223.34	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.129		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1626.00		NIST Webbook
tb	626.85	K	Joback Method
tc	834.90	K	Joback Method
tf	341.04	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.32	J/mol×K	626.85	Joback Method
cpg	543.41	J/mol×K	800.22	Joback Method
cpg	531.13	J/mol×K	765.55	Joback Method
cpg	518.03	J/mol×K	730.87	Joback Method
cpg	504.05	J/mol×K	696.20	Joback Method
cpg	489.16	J/mol×K	661.52	Joback Method
cpg	554.89	J/mol×K	834.90	Joback Method
dvisc	0.0001300	Pa×s	626.85	Joback Method

dvisc	0.0001691	Pa×s	579.22	Joback Method
dvisc	0.0002307	Pa×s	531.58	Joback Method
dvisc	0.0003345	Pa×s	483.95	Joback Method
dvisc	0.0005261	Pa×s	436.31	Joback Method
dvisc	0.0009243	Pa×s	388.68	Joback Method
dvisc	0.0019011	Pa×s	341.04	Joback Method

Sources

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=U131737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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