1-Heptanol, 2-(phenylmethylene)-, acetate

Other names:	Cinnamyl alcohol, «alpha»-pentyl-, acetate
	Amyl cinnamic acetate
	«alpha»-n-Amyl-«beta»-phenylacryl acetate
	«alpha»-Pentyl cinnamyl acetate
	«alpha»-N-Amyl cinnamyl acetate
	2-Pentyl-3-phenyl-2-propenyl acetate
	«alpha»-Amylcinnamyl acetate
	2-(phenylmethylene)heptyl acetate
Inchi:	InChI=1S/C16H22O2/c1-3-4-6-11-16(13-18-14(2)17)12-15-9-7-5-8-10-15/h5,7-10,12H,3-
InchiKey:	CMJSVJIGLBDCME-VBKFSLOCSA-N
Formula:	C16H22O2
SMILES:	CCCCCC(=Cc1ccccc1)COC(C)=O
Mol. weight [g/mol]:	246.34
CAS:	7493-78-9

Physical Properties

Property code	Value	Unit	Source
gf	34.00	kJ/mol	Joback Method
hf	-274.41	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.213		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1757.00		NIST Webbook
ripol	2318.00		NIST Webbook
ripol	2318.00		NIST Webbook
tb	672.49	K	Joback Method
tc	877.77	K	Joback Method
tf	349.62	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.73	J/mol×K	672.49	Joback Method
cpg	594.64	J/mol×K	706.70	Joback Method
cpg	610.54	J/mol×K	740.92	Joback Method
cpg	625.48	J/mol×K	775.13	Joback Method
cpg	639.50	J/mol×K	809.34	Joback Method
cpg	652.65	J/mol×K	843.56	Joback Method
cpg	664.97	J/mol×K	877.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7493789&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume