

2-Propen-1-ol, 3-phenyl-, acetate, (E)-

Other names:	(2E)-3-Phenyl-2-propenyl acetate (E)-Cinnamyl acetate trans-Cinnamyl acetate Cinnamyl alcohol, acetate, (E)-
Inchi:	InChI=1S/C11H12O2/c1-10(12)13-9-5-8-11-6-3-2-4-7-11/h2-8H,9H2,1H3/b8-5+
InchiKey:	WJSDHUCWMSHDCR-VMPITWQZSA-N
Formula:	C11H12O2
SMILES:	CC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	176.21
CAS:	21040-45-9

Physical Properties

Property code	Value	Unit	Source
gf	0.45	kJ/mol	Joback Method
hf	-161.42	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.263		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1414.00		NIST Webbook

rropol	1430.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	558.21	K	Joback Method
tc	776.95	K	Joback Method
tf	307.23	K	Joback Method
vc	0.547	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.27	J/mol×K	558.21	Joback Method
cpg	341.18	J/mol×K	594.67	Joback Method
cpg	354.22	J/mol×K	631.12	Joback Method
cpg	366.41	J/mol×K	667.58	Joback Method
cpg	377.80	J/mol×K	704.04	Joback Method
cpg	388.43	J/mol×K	740.50	Joback Method
cpg	398.33	J/mol×K	776.95	Joback Method
dvisc	0.0021241	Paxs	307.23	Joback Method
dvisc	0.0010842	Paxs	349.06	Joback Method
dvisc	0.0006391	Paxs	390.89	Joback Method
dvisc	0.0004172	Paxs	432.72	Joback Method
dvisc	0.0002937	Paxs	474.55	Joback Method
dvisc	0.0002188	Paxs	516.38	Joback Method
dvisc	0.0001704	Paxs	558.21	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=C21040459&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	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

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