

2-PENTEN-1-OL, ACETATE, (Z)-

Other names:	(2Z)-2-Pentenyl acetate (Z)-2-Pentenyl acetate (Z)-Pent-2-en-1-yl acetate 2-Penten-1-ol, acetate, (2Z)- cis-2-Penten-1-ol, acetate
Inchi:	InChI=1S/C7H12O2/c1-3-4-5-6-9-7(2)8/h4-5H,3,6H2,1-2H3
InchiKey:	WGGJTPQHVFQGN-PLNGDYQASA-N
Formula:	C7H12O2
SMILES:	CC/C=C\COC(C)=O
Mol. weight [g/mol]:	128.17

Physical Properties

Property code	Value	Unit	Source
af	0.3767		Cheméo Relay (1.0)
gf	-145.64	kJ/mol	Joback Method
hf	-412.59	kJ/mol	Cheméo Relay (1.0)
hfus	16.88	kJ/mol	Joback Method
hvap	46.71	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-1.61		Cheméo Relay (1.0)
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	908.70		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	897.00		NIST Webbook
tb	416.17	K	Cheméo Relay (1.0)
tc	590.63	K	Cheméo Relay (1.0)
tf	175.80	K	Cheméo Relay (1.0)
vc	0.407	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	222.68	J/mol×K	440.01	Joback Method
cpg	233.44	J/mol×K	470.85	Joback Method
cpg	243.76	J/mol×K	501.68	Joback Method
cpg	253.64	J/mol×K	532.52	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0029377	Pa×s	235.73	Joback Method
dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0002208	Pa×s	440.01	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C42125100&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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