

1,6-Heptadien-4-ol, acetate

Inchi:	InChI=1S/C9H14O2/c1-4-6-9(7-5-2)11-8(3)10/h4-5,9H,1-2,6-7H2,3H3
InchiKey:	GGOHGGVWCJPFTK-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	C=CCC(CC=C)OC(C)=O
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
gf	-35.78	kJ/mol	Joback Method
hf	-228.31	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.070		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
tb	474.53	K	Joback Method
tc	658.99	K	Joback Method
tf	244.83	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.35	J/molxK	474.53	Joback Method
cpg	345.19	J/molxK	628.25	Joback Method
cpg	334.85	J/molxK	597.50	Joback Method
cpg	324.01	J/molxK	566.76	Joback Method
cpg	312.66	J/molxK	536.02	Joback Method
cpg	300.77	J/molxK	505.27	Joback Method
cpg	355.04	J/molxK	658.99	Joback Method
dvisc	0.0002316	Paxs	474.53	Joback Method

dvisc	0.0003019	Paxs	436.25	Joback Method
dvisc	0.0004142	Paxs	397.96	Joback Method
dvisc	0.0006077	Paxs	359.68	Joback Method
dvisc	0.0009770	Paxs	321.40	Joback Method
dvisc	0.0017860	Paxs	283.11	Joback Method
dvisc	0.0039424	Paxs	244.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352756&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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