

2-Methyl-3-butenyl acetate

Inchi:	InChI=1S/C7H12O2/c1-4-6(2)5-9-7(3)8/h4,6H,1,5H2,2-3H3
InchiKey:	BRFRRYWRNMHZJE-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CC(C)COC(C)=O
Mol. weight [g/mol]:	128.17

Physical Properties

Property code	Value	Unit	Source
gf	-140.46	kJ/mol	Joback Method
hf	-312.46	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
ripol	1199.00		NIST Webbook
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tb	432.09	K	Joback Method
tc	616.21	K	Joback Method
tf	224.05	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.93	J/molxK	432.09	Joback Method
cpg	233.73	J/molxK	462.78	Joback Method
cpg	244.12	J/molxK	493.46	Joback Method
cpg	254.10	J/molxK	524.15	Joback Method
cpg	263.67	J/molxK	554.84	Joback Method
cpg	272.85	J/molxK	585.52	Joback Method
cpg	281.64	J/molxK	616.21	Joback Method
dvisc	0.0042260	Paxs	224.05	Joback Method

dvisc	0.0019297	Paxs	258.72	Joback Method
dvisc	0.0010605	Paxs	293.40	Joback Method
dvisc	0.0006615	Paxs	328.07	Joback Method
dvisc	0.0004515	Paxs	362.74	Joback Method
dvisc	0.0003294	Paxs	397.42	Joback Method
dvisc	0.0002529	Paxs	432.09	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=R600205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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