2-Methylbut-2-en-1-yl acetate

Inchi: InChI=1S/C7H12O2/c1-4-6(2)5-9-7(3)8/h4H,5H2,1-3H3/b6-4+
InchiKey: LYFIKZOWBKYNSE-GQCTYLIASA-N
Formula: C7H12O2
SMILES: CC=C(C)COC(C)=O
Mol. weight [g/mol]: 128.17
CAS: 33425-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	921.40		NIST Webbook
rinpol	921.40		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1232.00		NIST Webbook
tb	439.89	K	Joback Method
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/mol×K	439.89	Joback Method
cpg	233.55	J/mol×K	471.32	Joback Method
cpg	244.02	J/mol×K	502.76	Joback Method

cpg	254.05	J/mol×K	534.19	Joback Method
cpg	263.64	J/mol×K	565.63	Joback Method
cpg	272.80	J/mol×K	597.06	Joback Method
cpg	281.54	J/mol×K	628.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33425308&Units=SI

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