

2-Propen-1-ol, 2-methyl-, acetate

Other names:	Methallyl acetate «beta»-Methallyl acetate 1-Acetoxy-2-methyl-2-propene 2-Methylallyl acetate Acetic acid, 2-methylallylester Ir_5525 Ir
Inchi:	InChI=1S/C6H10O2/c1-5(2)4-8-6(3)7/h1,4H2,2-3H3
InchiKey:	IVKYUXHYUAMPMT-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=C(C)COC(C)=O
Mol. weight [g/mol]:	114.14
CAS:	820-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-154.99	kJ/mol	Joback Method
hf	-296.33	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	409.53	K	Joback Method
tc	594.44	K	Joback Method
tf	213.82	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.88	J/mol×K	409.53	Joback Method
cpg	194.21	J/mol×K	440.35	Joback Method

cpg	203.19	J/mol×K	471.17	Joback Method
cpg	211.85	J/mol×K	501.99	Joback Method
cpg	220.17	J/mol×K	532.81	Joback Method
cpg	228.17	J/mol×K	563.63	Joback Method
cpg	235.83	J/mol×K	594.44	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=C820713&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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