2,2-Dimethylpropanoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C13H24O2/c1-6-7-8-9-10-11(2)15-12(14)13(3,4)5/h9-11H,6-8H2,1-5H3/b10-9+
InchiKey: CIYFYDOFPMJDQX-MDZDMXLPSA-N
Formula: C13H24O2
SMILES: CCCCC=CC(C)OC(=O)C(C)(C)C
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-94.72	kJ/mol	Joback Method
hf	-453.26	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.711		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1268.00		NIST Webbook
tb	573.62	K	Joback Method
tc	761.27	K	Joback Method
tf	290.77	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.07	J/mol×K	573.62	Joback Method
cpg	576.38	J/mol×K	730.00	Joback Method
cpg	562.54	J/mol×K	698.72	Joback Method
cpg	547.93	J/mol×K	667.45	Joback Method
cpg	532.50	J/mol×K	636.17	Joback Method
cpg	516.23	J/mol×K	604.90	Joback Method
cpg	589.47	J/mol×K	761.27	Joback Method
dvisc	0.0001233	Pa×s	573.62	Joback Method
dvisc	0.0001727	Pa×s	526.48	Joback Method

dvisc	0.0002584	Pa×s	479.34	Joback Method
dvisc	0.0004222	Pa×s	432.19	Joback Method
dvisc	0.0007778	Pa×s	385.05	Joback Method
dvisc	0.0016996	Pa×s	337.91	Joback Method
dvisc	0.0047852	Pa×s	290.77	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=U299333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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