1-Ethenyl-7-methyloctyl Prop-2-enoate

Inchi: InChI=1S/C14H24O2/c1-5-13(16-14(15)6-2)11-9-7-8-10-12(3)4/h5-6,12-13H,1-2,7-11H2,
InchiKey: SDKFPARMEUMSPM-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: C=CC(=O)OC(C=C)CCCCCC(C)C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	3.88	kJ/mol	Joback Method
hf	-336.79	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	53.80	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.877		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
tb	588.49	K	Joback Method
tc	767.54	K	Joback Method
tf	286.18	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.23	J/mol×K	588.49	Joback Method
cpg	541.78	J/mol×K	618.33	Joback Method
cpg	557.57	J/mol×K	648.17	Joback Method
cpg	572.61	J/mol×K	678.02	Joback Method
cpg	586.94	J/mol×K	707.86	Joback Method
cpg	600.56	J/mol×K	737.70	Joback Method
cpg	613.50	J/mol×K	767.54	Joback Method
dvisc	0.0047061	Pa×s	286.18	Joback Method

dvisc	0.0017037	Pa×s	336.56	Joback Method
dvisc	0.0008036	Pa×s	386.95	Joback Method
dvisc	0.0004507	Pa×s	437.34	Joback Method
dvisc	0.0002849	Pa×s	487.72	Joback Method
dvisc	0.0001962	Pa×s	538.11	Joback Method
dvisc	0.0001440	Pa×s	588.49	Joback Method

Sources

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=R412607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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