1-Ethenyl-7-methylnonyl Prop-2-enoate

Inchi: InChI=1S/C15H26O2/c1-5-13(4)11-9-8-10-12-14(6-2)17-15(16)7-3/h6-7,13-14H,2-3,5,8-1
InchiKey: TWXJMPDHSKXVID-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C=CC(=O)OC(C=C)CCCCCC(C)CC
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	12.30	kJ/mol	Joback Method
hf	-357.43	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.267		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1552.00		NIST Webbook
tb	611.37	K	Joback Method
tc	789.05	K	Joback Method
tf	297.45	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.55	J/mol×K	611.37	Joback Method
cpg	594.60	J/mol×K	640.98	Joback Method
cpg	610.86	J/mol×K	670.60	Joback Method
cpg	626.36	J/mol×K	700.21	Joback Method
cpg	641.10	J/mol×K	729.82	Joback Method
cpg	655.12	J/mol×K	759.43	Joback Method
cpg	668.44	J/mol×K	789.05	Joback Method
dvisc	0.0043488	Pa×s	297.45	Joback Method
dvisc	0.0015618	Pa×s	349.77	Joback Method

dvisc	0.0007321	Pa×s	402.09	Joback Method
dvisc	0.0004086	Pa×s	454.41	Joback Method
dvisc	0.0002573	Pa×s	506.73	Joback Method
dvisc	0.0001766	Pa×s	559.05	Joback Method
dvisc	0.0001293	Pa×s	611.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R412598&Units=SI

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

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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