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	655.12	J/mol×K	759.43	Joback Method
cpg	641.10	J/mol×K	729.82	Joback Method
cpg	626.36	J/mol×K	700.21	Joback Method
cpg	610.86	J/mol×K	670.60	Joback Method
cpg	594.60	J/mol×K	640.98	Joback Method
cpg	668.44	J/mol×K	789.05	Joback Method
dvisc	0.0001293	Pa×s	611.37	Joback Method
dvisc	0.0001766	Pa×s	559.05	Joback Method

dvisc	0.0002573	Pa×s	506.73	Joback Method
dvisc	0.0004086	Pa×s	454.41	Joback Method
dvisc	0.0007321	Pa×s	402.09	Joback Method
dvisc	0.0015618	Pa×s	349.77	Joback Method
dvisc	0.0043488	Pa×s	297.45	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=R412598&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

Latest version available from:
https://www.chemeo.com/cid/34-691-7/1-Ethenyl-7-methylnonyl-Prop-2-enoate.pdf
Generated by Cheméo on 2024-10-12 05:36:04.89775272 +0000 UTC m=+3292227.534721979.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.