(E)-2-Hexenyl-(E)-7,9-decadienoate

Inchi: InChI=1S/C16H26O2/c1-3-5-7-9-10-11-12-14-16(17)18-15-13-8-6-4-2/h3,5,7-8,13H,1,4,6
InchiKey: SBTGHFZCYIFQIH-OAPZVAQESA-N
Formula: C16H26O2
SMILES: C=CC=CCCCCCC(=O)OCC=CCCC
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	98.20	kJ/mol	Joback Method
hf	-258.50	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.579		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	646.77	K	Joback Method
tc	827.09	K	Joback Method
tf	330.32	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.35	J/mol×K	646.77	Joback Method
cpg	686.42	J/mol×K	797.03	Joback Method
cpg	672.86	J/mol×K	766.98	Joback Method
cpg	658.62	J/mol×K	736.93	Joback Method
cpg	643.64	J/mol×K	706.88	Joback Method
cpg	627.90	J/mol×K	676.82	Joback Method
cpg	699.31	J/mol×K	827.09	Joback Method
dvisc	0.0000942	Pa×s	646.77	Joback Method

dvisc	0.0001252	Pa×s	594.03	Joback Method
dvisc	0.0001758	Pa×s	541.29	Joback Method
dvisc	0.0002658	Pa×s	488.54	Joback Method
dvisc	0.0004442	Pa×s	435.80	Joback Method
dvisc	0.0008550	Pa×s	383.06	Joback Method
dvisc	0.0020284	Pa×s	330.32	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=R556599&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