

(E)-Methyl 7,9-decadienoate

Inchi:	InChI=1S/C11H18O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-5H,1,6-10H2,2H3/b5-4+
InchiKey:	ZVRIADBQUBCHBH-SNAWJCMRSA-N
Formula:	C11H18O2
SMILES:	C=CC=CCCCCCC(=O)OC
Mol. weight [g/mol]:	182.26

Physical Properties

Property code	Value	Unit	Source
gf	-24.12	kJ/mol	Joback Method
hf	-272.52	kJ/mol	Joback Method
hfus	25.96	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1350.00		NIST Webbook
tb	528.21	K	Joback Method
tc	709.59	K	Joback Method
tf	279.05	K	Joback Method
vc	0.636	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.28	J/mol×K	528.21	Joback Method
cpg	392.34	J/mol×K	558.44	Joback Method
cpg	405.76	J/mol×K	588.67	Joback Method
cpg	418.57	J/mol×K	618.90	Joback Method
cpg	430.77	J/mol×K	649.13	Joback Method
cpg	442.39	J/mol×K	679.36	Joback Method
cpg	453.46	J/mol×K	709.59	Joback Method
dvisc	0.0027775	Paxs	279.05	Joback Method
dvisc	0.0013060	Paxs	320.58	Joback Method

dvisc	0.0007301	Paxs	362.10	Joback Method
dvisc	0.0004600	Paxs	403.63	Joback Method
dvisc	0.0003160	Paxs	445.16	Joback Method
dvisc	0.0002314	Paxs	486.68	Joback Method
dvisc	0.0001779	Paxs	528.21	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=R556608&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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