

2,4-Decadienoic acid, methyl ester, (Z,E)-

Other names:	Methyl 2,4-trans,cis-decadienoate Methyl 2,4 (Z,E)-decadienoate
Inchi:	InChI=1S/C11H18O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h7-10H,3-6H2,1-2H3/b8-7+,10-9-
InchiKey:	SFHSEXGIVSBRRK-GOJKSUSPSA-N
Formula:	C11H18O2
SMILES:	CCCCC=CC=CC(=O)OC
Mol. weight [g/mol]:	182.26
CAS:	108965-84-0

Physical Properties

Property code	Value	Unit	Source
gf	-31.74	kJ/mol	Joback Method
hf	-280.73	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mvol	164.690	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1332.00		NIST Webbook
ripol	1768.00		NIST Webbook
tb	535.69	K	Joback Method
tc	721.31	K	Joback Method
tf	275.73	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.20	J/mol×K	535.69	Joback Method
cpg	393.43	J/mol×K	566.63	Joback Method
cpg	406.97	J/mol×K	597.56	Joback Method
cpg	419.86	J/mol×K	628.50	Joback Method
cpg	432.12	J/mol×K	659.44	Joback Method

cpg	443.78	J/molxK	690.38	Joback Method
cpg	454.86	J/molxK	721.31	Joback Method
dvisc	0.0027700	Paxs	275.73	Joback Method
dvisc	0.0012188	Paxs	319.06	Joback Method
dvisc	0.0006526	Paxs	362.38	Joback Method
dvisc	0.0003993	Paxs	405.71	Joback Method
dvisc	0.0002686	Paxs	449.04	Joback Method
dvisc	0.0001938	Paxs	492.36	Joback Method
dvisc	0.0001473	Paxs	535.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108965840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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