methyl 2,4-decadienoate

Other names: methyl (2E,4E)-2,4-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-XBLVEGMJSA-N
Formula: C11H18O2
SMILES: CCCCCC=CC=CC(=O)OC
Mol. weight [g/mol]: 182.26
CAS: 7328-33-8

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
mcvol	164.690	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1819.00		NIST Webbook
tb	535.69	K	Joback Method
tc	721.31	K	Joback Method
tf	275.73	K	Joback Method
vc	0.635	m3/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/mol×K	690.38	Joback Method
cpg	454.86	J/mol×K	721.31	Joback Method
dvisc	0.0027700	Pa×s	275.73	Joback Method
dvisc	0.0012188	Pa×s	319.06	Joback Method
dvisc	0.0006526	Pa×s	362.38	Joback Method
dvisc	0.0003993	Pa×s	405.71	Joback Method
dvisc	0.0002686	Pa×s	449.04	Joback Method
dvisc	0.0001938	Pa×s	492.36	Joback Method
dvisc	0.0001473	Pa×s	535.69	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=C7328338&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume