

Ethyl 2,4-dimethyl-2,4-hexadienoate, not E,E, # 1

Inchi:	InChI=1S/C8H12O2/c1-3-5-6-7-8(9)10-4-2/h3,5-7H,4H2,1-2H3
InchiKey:	OZZYKXXGCOLLLO-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC=CC=CC(=O)OCC
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
gf	-57.00	kJ/mol	Joback Method
hf	-218.81	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	42.47	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.682		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinsol	1140.00		NIST Webbook
tb	467.05	K	Joback Method
tc	659.15	K	Joback Method
tf	241.92	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.65	J/molxK	467.05	Joback Method
cpg	258.15	J/molxK	499.07	Joback Method
cpg	269.08	J/molxK	531.08	Joback Method
cpg	279.46	J/molxK	563.10	Joback Method
cpg	289.32	J/molxK	595.12	Joback Method
cpg	298.68	J/molxK	627.13	Joback Method
cpg	307.56	J/molxK	659.15	Joback Method
dvisc	0.0028027	Paxs	241.92	Joback Method
dvisc	0.0012997	Paxs	279.44	Joback Method

dvisc	0.0007230	Paxs	316.96	Joback Method
dvisc	0.0004553	Paxs	354.49	Joback Method
dvisc	0.0003133	Paxs	392.01	Joback Method
dvisc	0.0002301	Paxs	429.53	Joback Method
dvisc	0.0001776	Paxs	467.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R597807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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