2,4-Hexadienoic acid, ethyl ester, (2E,4E)-

Other names:	Sorbic acid, ethyl ester
	Ethyl sorbate
	Ethyl 2,4-hexadienoate, (E,E)-
	2,4-Hexadienoic acid, ethyl ester, (E,E)-
	Ethylhexa-2,4-dienoate, (trans,trans)-
	(E,E)-Ethyl 2,4-hexadienoate
	Ethyl (2E,4E)-2,4-hexadienoate
	(E,E)-2,4-hexadienoic acid ethyl ester
	NSC 8874
	2,4-Hexadienoic acid, ethyl ester
	Ethyl 2,4-hexadienoate
	Ethyl hexa-2,4-dienoate
Inchi:	InChI=1S/C8H12O2/c1-3-5-6-7-8(9)10-4-2/h3,5-7H,4H2,1-2H3/b5-3+,7-6+
InchiKey:	OZZYKXXGCOLLLO-TWTPFVCWSA-N
Formula:	C8H12O2
SMILES:	CC=CC=CC(=O)OCC
Mol. weight [g/mol]:	140.18
CAS:	2396-84-1

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
rinpol	1067.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook

rinpol	1089.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1093.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	468.70	K	NIST Webbook
tc	659.15	K	Joback Method
tf	241.92	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.65	J/mol×K	467.05	Joback Method
cpg	298.68	J/mol×K	627.13	Joback Method
cpg	289.32	J/mol×K	595.12	Joback Method
cpg	279.46	J/mol×K	563.10	Joback Method
cpg	269.08	J/mol×K	531.08	Joback Method
cpg	258.15	J/mol×K	499.07	Joback Method
cpg	307.56	J/mol×K	659.15	Joback Method
dvisc	0.0001776	Pa×s	467.05	Joback Method
dvisc	0.0002301	Pa×s	429.53	Joback Method
dvisc	0.0003133	Pa×s	392.01	Joback Method
dvisc	0.0004553	Pa×s	354.49	Joback Method
dvisc	0.0007230	Pa×s	316.96	Joback Method
dvisc	0.0012997	Pa×s	279.44	Joback Method
dvisc	0.0028027	Pa×s	241.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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