

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

Other names:

Ethyl trans,cis-2,4-decadienoate
Ethyl (E,Z)-2,4-decadienoate
Ethyl trans-2,cis-4-decadienoate
Ethyl (2E,4Z)-decadienoate
Ethyl 2,4 (E,Z)-decadienoate
Ethyl-deca-(2E,4Z)-dienoate
Ethyl (E)-2,(Z)-4-decadienoate
ethyl 2,4-decadienoate
ethyl (2E,4Z)-2,4-decadienoate

Inchi:

InChI=1S/C12H20O2/c1-3-5-6-7-8-9-10-11-12(13)14-4-2/h8-11H,3-7H2,1-2H3/b9-8+,11-

InchiKey:

OPCRGEVPIBLWAY-BNFZFUHLSA-N

Formula:

C12H20O2

SMILES:

CCCCC=CC=CC(=O)OCC

Mol. weight [g/mol]:

196.29

CAS:

3025-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.32	kJ/mol	Joback Method
hf	-301.37	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1444.00		NIST Webbook

ripol	1449.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1818.00		NIST Webbook
tb	558.57	K	Joback Method
tc	742.19	K	Joback Method
tf	287.00	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.05	J/molxK	558.57	Joback Method
cpg	441.98	J/molxK	589.17	Joback Method
cpg	456.20	J/molxK	619.78	Joback Method
cpg	469.73	J/molxK	650.38	Joback Method
cpg	482.61	J/molxK	680.98	Joback Method
cpg	494.87	J/molxK	711.59	Joback Method
cpg	506.52	J/molxK	742.19	Joback Method
dvisc	0.0026769	Paxs	287.00	Joback Method
dvisc	0.0011604	Paxs	332.26	Joback Method
dvisc	0.0006146	Paxs	377.52	Joback Method
dvisc	0.0003730	Paxs	422.79	Joback Method
dvisc	0.0002493	Paxs	468.05	Joback Method
dvisc	0.0001789	Paxs	513.31	Joback Method
dvisc	0.0001355	Paxs	558.57	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3025307&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
mccvol: 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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