

Ethyl 2,4-decadienoate

Other names:	Ethyl 2,4 (E,E)-decadienoate ethyl (E)-2,(E)-4-decadienoate ethyl (2E,4E)-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:	7328-34-9

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	1445.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1465.00		NIST Webbook
tb	558.57	K	Joback Method
tc	742.19	K	Joback Method
tf	287.00	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.05	J/mol×K	558.57	Joback Method
cpg	441.98	J/mol×K	589.17	Joback Method
cpg	456.20	J/mol×K	619.78	Joback Method
cpg	469.73	J/mol×K	650.38	Joback Method
cpg	482.61	J/mol×K	680.98	Joback Method
cpg	494.87	J/mol×K	711.59	Joback Method
cpg	506.52	J/mol×K	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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7328349&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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