

5,8,11,14-Eicosatetraenoic acid, ethyl ester

Other names:	5,8,11,14-eicosatetraenoic acid, ethyl ester, (all-Z)-
Inchi:	InChI=1S/C22H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24-4-2
InchiKey:	SNXPWYFWAZVIAU-GKFFVBPDJSA-N
Formula:	C22H36O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCCC(=O)OCC
Mol. weight [g/mol]:	332.52
CAS:	95285-77-1

Physical Properties

Property code	Value	Unit	Source
gf	221.32	kJ/mol	Joback Method
hf	-273.33	kJ/mol	Joback Method
hfus	56.33	kJ/mol	Joback Method
hvap	73.55	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.695		Crippen Method
mcvol	311.080	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
tb	795.69	K	Joback Method
tc	983.56	K	Joback Method
tf	389.54	K	Joback Method
vc	1.212	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.00	J/molxK	795.69	Joback Method
cpg	951.44	J/molxK	827.00	Joback Method
cpg	969.02	J/molxK	858.31	Joback Method
cpg	985.79	J/molxK	889.62	Joback Method
cpg	1001.82	J/molxK	920.94	Joback Method
cpg	1017.20	J/molxK	952.25	Joback Method
cpg	1031.98	J/molxK	983.56	Joback Method
dvisc	0.0010302	Paxs	389.54	Joback Method

dvisc	0.0003755	Paxs	457.23	Joback Method
dvisc	0.0001776	Paxs	524.92	Joback Method
dvisc	0.0000997	Paxs	592.62	Joback Method
dvisc	0.0000630	Paxs	660.31	Joback Method
dvisc	0.0000433	Paxs	728.00	Joback Method
dvisc	0.0000318	Paxs	795.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Binary Diffusion Coefficients of Arachidonic Acid Ethyl Esters, Eicosapentaenoic Acid Ethyl Esters, and Docosahexaenoic Acid Ethyl Esters in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060456h
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=C95285771&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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