

5,8,11,14-Eicosatetraenoic acid, methyl ester, (all-Z)-

Other names:

5,8,11,14-Eicosatetraenoic acid, methyl ester
5,8,11,14-Eicosatetraenoic acid, methyl ester, cis-
Arachidonic acid methyl ester
Methyl Z,Z,Z,Z 5,8,11,14-eicosatetraeneoate
Methyl all-cis-5,8,11,14-eicosatetraenoate
Methyl arachidonate
cis-5,8,11,14-Eicosatetraenoic acid, methyl ester
methyl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate

Inchi: InChI=1S/C21H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h

InchiKey: OFIDNKMQBYPYGNW-ZKWNWVNESA-N

Formula: C₂₁H₃₄O₂

SMILES: CCCCCC=CCC=CCC=CCC=CCCCC(=O)OC

Mol. weight [g/mol]: 318.49

CAS: 2566-89-4

Physical Properties

Property code	Value	Unit	Source
gf	212.90	kJ/mol	Joback Method
hf	-252.69	kJ/mol	Joback Method
hfus	53.74	kJ/mol	Joback Method
h _{vap}	118.30	kJ/mol	NIST Webbook
h _{vap}	122.60 ± 1.60	kJ/mol	NIST Webbook
log ₁₀ ws	-6.89		Crippen Method
logp	6.305		Crippen Method
m _{cvol}	296.990	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2274.40		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	772.81	K	Joback Method
tc	959.66	K	Joback Method
tf	378.27	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.07	J/molxK	959.66	Joback Method
cpg	955.68	J/molxK	928.52	Joback Method
cpg	940.69	J/molxK	897.38	Joback Method
cpg	925.03	J/molxK	866.24	Joback Method
cpg	908.65	J/molxK	835.09	Joback Method
cpg	891.46	J/molxK	803.95	Joback Method
cpg	873.42	J/molxK	772.81	Joback Method
dvisc	0.0011500	Paxs	378.27	Joback Method
dvisc	0.0000363	Paxs	772.81	Joback Method
dvisc	0.0000494	Paxs	707.05	Joback Method
dvisc	0.0000716	Paxs	641.30	Joback Method
dvisc	0.0001129	Paxs	575.54	Joback Method
dvisc	0.0002005	Paxs	509.78	Joback Method
dvisc	0.0004220	Paxs	444.03	Joback Method
hvapt	118.30	kJ/mol	298.15	the vaporization enthalpies and vapor pressures of a series of unstaured fatty acid methyl esters by correlation gas chromatography

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2566894&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

the vaporization enthalpies and vapor pressures of a series of unstaured fatty acid methyl esters by correlation gas chromatography:

<https://www.doi.org/10.1016/j.tca.2007.02.008>

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
hvapt:	Enthalpy of vaporization at a given temperature
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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