5,8,11,14,17-Eicosapentaenoic acid, methyl ester

Inchi: InChI=1S/C22H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24-2
InchiKey: CLBWGVLBIKYNAZ-LRKAYDMASA-N
Formula: C22H34O2
SMILES: CCCC=CCC=CCC=CCC=CCC=CCCCC(=O)OC
Mol. weight [g/mol]: 330.50

Physical Properties

Property code	Value	Unit	Source
gf	301.54	kJ/mol	Joback Method
hf	-156.11	kJ/mol	Joback Method
hfus	56.53	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.471		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook
tb	799.85	K	Joback Method
tc	991.48	K	Joback Method
tf	384.46	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.96	J/mol×K	799.85	Joback Method
cpg	925.94	J/mol×K	831.79	Joback Method
cpg	943.09	J/mol×K	863.73	Joback Method
cpg	959.50	J/mol×K	895.66	Joback Method
cpg	975.25	J/mol×K	927.60	Joback Method
cpg	990.42	J/mol×K	959.54	Joback Method
cpg	1005.10	J/mol×K	991.48	Joback Method

dvisc	0.0009665	Pa×s	384.46	Joback Method
dvisc	0.0003401	Pa×s	453.69	Joback Method
dvisc	0.0001578	Pa×s	522.92	Joback Method
dvisc	0.0000876	Pa×s	592.15	Joback Method
dvisc	0.0000550	Pa×s	661.39	Joback Method
dvisc	0.0000377	Pa×s	730.62	Joback Method
dvisc	0.0000276	Pa×s	799.85	Joback Method

Sources

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=R98775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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