Methyl 7,10,13,16,19-docosapentaenoate

Other names: 7,10,13,16,19-docosapentaenoic acid, methyl ester
Inchi: InChI=1S/C23H36O2/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: PTFHIRHGARALFY-JEBPEJKESA-N
Formula: C23H36O2
SMILES: CCC=CCC=CCC=CCC=CCC=CCCCCCC(=O)OC
Mol. weight [g/mol]: 344.53

Physical Properties

Property code	Value	Unit	Source
gf	309.96	kJ/mol	Joback Method
hf	-176.75	kJ/mol	Joback Method
hfus	59.12	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.861		Crippen Method
mcvol	320.870	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	822.73	K	Joback Method
tc	1015.51	K	Joback Method
tf	395.73	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.98	J/mol×K	822.73	Joback Method
cpg	1052.64	J/mol×K	983.38	Joback Method
cpg	1037.01	J/mol×K	951.25	Joback Method
cpg	1020.82	J/mol×K	919.12	Joback Method
cpg	1003.97	J/mol×K	886.99	Joback Method
cpg	986.39	J/mol×K	854.86	Joback Method

cpg	1067.79	J/mol×K	1015.51	Joback Method
dvisc	0.0000242	Pa×s	822.73	Joback Method
dvisc	0.0000331	Pa×s	751.56	Joback Method
dvisc	0.0000483	Pa×s	680.40	Joback Method
dvisc	0.0000771	Pa×s	609.23	Joback Method
dvisc	0.0001394	Pa×s	538.06	Joback Method
dvisc	0.0003017	Pa×s	466.90	Joback Method
dvisc	0.0008620	Pa×s	395.73	Joback Method

Sources

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=U336508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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