

Docosahexaenoic acid, methyl ester

Inchi:	InChI=1S/C23H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)
InchiKey:	YGMKRBTWFPWWSX-SFGLVEFQSA-N
Formula:	C23H34O2
SMILES:	CC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)OC
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	390.18	kJ/mol	Joback Method
hf	-59.53	kJ/mol	Joback Method
hfus	59.32	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.637		Crippen Method
mvol	316.570	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
ripol	2413.00		NIST Webbook
ripol	2413.00		NIST Webbook
tb	826.89	K	Joback Method
tc	1023.30	K	Joback Method
tf	390.65	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.27	J/molxK	826.89	Joback Method
cpg	960.24	J/molxK	859.62	Joback Method
cpg	977.45	J/molxK	892.36	Joback Method
cpg	994.00	J/molxK	925.09	Joback Method
cpg	1010.00	J/molxK	957.83	Joback Method
cpg	1025.54	J/molxK	990.56	Joback Method
cpg	1040.72	J/molxK	1023.30	Joback Method
dvisc	0.0008093	Paxs	390.65	Joback Method

dvisc	0.0002734	Paxs	463.36	Joback Method
dvisc	0.0001240	Paxs	536.06	Joback Method
dvisc	0.0000679	Paxs	608.77	Joback Method
dvisc	0.0000423	Paxs	681.48	Joback Method
dvisc	0.0000289	Paxs	754.18	Joback Method
dvisc	0.0000211	Paxs	826.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R567970&Units=SI
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

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

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