Doconexent

Other names:	(all-Z)-4,7,10,13,16,19-Docosahexaenoic acid
	4,7,10,13,16,19-Docosahexaenoic acid
	4,7,10,13,16,19-Docosahexaenoic acid, (4Z,7Z,10Z,13Z,16Z,19Z)-
	4,7,10,13,16,19-Docosahexaenoic acid, (all cis)-
	4-cis,7-cis,10-cis,13-cis,16-cis,19-cis-Docosahexaenoic acid
	AquaGrow Advantage
	Cervonic acid
	DHA
	Docosahexaenoic acid
	Martek DHA HM
	Ropufa 60
	cis-4,7,10,13,16,19-Docosahexaenoic acid
	cis-4,7,10,13,16,19-Docosahexanoic acid
Inchi:	InChI=1S/C22H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24
InchiKey:	MBMBGCFOFBJSGT-KUBAVDMBSA-N
Formula:	C22H32O2
SMILES:	CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O
Mol. weight [g/mol]:	328.49
CAS:	6217-54-5

Physical Properties

Property code	Value	Unit	Source
gf	349.94	kJ/mol	Joback Method
hf	-58.90	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	87.74	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.549		Crippen Method
mcvol	302.480	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2520.90		NIST Webbook
rinpol	2520.90		NIST Webbook
tb	873.77	K	Joback Method
tc	1073.06	K	Joback Method
tf	417.97	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.10	J/mol×K	873.77	Joback Method
cpg	935.35	J/mol×K	906.99	Joback Method
cpg	951.09	J/mol×K	940.20	Joback Method
cpg	966.44	J/mol×K	973.42	Joback Method
cpg	981.52	J/mol×K	1006.63	Joback Method
cpg	996.45	J/mol×K	1039.85	Joback Method
cpg	1011.34	J/mol×K	1073.06	Joback Method
dvisc	0.0009411	Pa×s	417.97	Joback Method
dvisc	0.0002003	Pa×s	493.94	Joback Method
dvisc	0.0000644	Pa×s	569.90	Joback Method
dvisc	0.0000270	Pa×s	645.87	Joback Method
dvisc	0.0000136	Pa×s	721.84	Joback Method
dvisc	0.0000078	Pa×s	797.80	Joback Method
dvisc	0.0000049	Pa×s	873.77	Joback Method
hvapt	162.90	kJ/mol	298.15	Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids 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=C6217545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je5009729
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
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