cis-5,8,11,14,17-Eicosapentaenoic acid

Other names:	Icosapentaenoic acid
	(all-Z)-5,8,11,14,17-Eicosapentaenoic acid
	EPA
	Timnodonic acid
	5,8,11,14,17-Eicosapentaenoic acid, (5Z,8Z,11Z,14Z,17Z)-
	Eicosapentaenoic acid
Inchi:	InChI=1S/C20H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h3-4,
InchiKey:	JAZBEHYOTPTENJ-JLNKQSITSA-N
Formula:	C20H30O2
SMILES:	CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O
Mol. weight [g/mol]:	302.45
CAS:	10417-94-4

Physical Properties

Property code	Value	Unit	Source
gf	252.88	kJ/mol	Joback Method
hf	-134.84	kJ/mol	Joback Method
hfus	54.25	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.993		Crippen Method
mcvol	278.600	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2334.20		NIST Webbook
rinpol	2334.20		NIST Webbook
tb	823.85	K	Joback Method
tc	1015.83	K	Joback Method
tf	400.51	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.37	J/mol×K	823.85	Joback Method

cpg	842.80	J/mol×K	855.85	Joback Method
cpg	857.60	J/mol×K	887.84	Joback Method
cpg	871.88	J/mol×K	919.84	Joback Method
cpg	885.71	J/mol×K	951.83	Joback Method
cpg	899.21	J/mol×K	983.83	Joback Method
cpg	912.45	J/mol×K	1015.83	Joback Method
dvisc	0.0014454	Pa×s	400.51	Joback Method
dvisc	0.0003190	Pa×s	471.07	Joback Method
dvisc	0.0001043	Pa×s	541.62	Joback Method
dvisc	0.0000442	Pa×s	612.18	Joback Method
dvisc	0.0000223	Pa×s	682.74	Joback Method
dvisc	0.0000128	Pa×s	753.29	Joback Method
dvisc	0.0000081	Pa×s	823.85	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10417944&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume