METHYL EICOSA-5,8,11,14,17-PENTAENOATE

Other names: Eicosapentaenoic acid, methyl ester
Inchi: InChI=1S/C21H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h4
InchiKey: QWDCYFDDFPWISL-ZACMJQCDSA-N
Formula: C21H32O2
SMILES: CC/C=C/C/C=C/C/C=C/C/C=C/C/C=C/CCCC(=O)OC
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
af	0.5247		Cheméo Relay (1.0)
hf	-386.14	kJ/mol	Cheméo Relay (1.0)
hfus	53.94	kJ/mol	Joback Method
hvap	121.45	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-6.06		Cheméo Relay (1.0)
logp	6.081		Crippen Method
mcvol	292.690	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
ripol	2174.00		NIST Webbook
ripol	2174.00		NIST Webbook
tb	591.19	K	Cheméo Relay (1.0)
tc	776.89	K	Cheméo Relay (1.0)
tf	295.30	K	Cheméo Relay (1.0)
vc	0.943	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.88	J/mol×K	776.97	Joback Method
cpg	866.46	J/mol×K	808.82	Joback Method
cpg	883.21	J/mol×K	840.68	Joback Method
cpg	899.21	J/mol×K	872.53	Joback Method
cpg	914.55	J/mol×K	904.39	Joback Method
cpg	929.29	J/mol×K	936.24	Joback Method

cpg	943.52	J/mol×K	968.10	Joback Method
dvisc	0.0010789	Pa×s	373.19	Joback Method
dvisc	0.0003818	Pa×s	440.49	Joback Method
dvisc	0.0001780	Pa×s	507.78	Joback Method
dvisc	0.0000992	Pa×s	575.08	Joback Method
dvisc	0.0000625	Pa×s	642.38	Joback Method
dvisc	0.0000430	Pa×s	709.67	Joback Method
dvisc	0.0000315	Pa×s	776.97	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191657&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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