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: CCC=CCC=CCC=CCC=CCC=CCCCC(=O)OC
Mol. weight [g/mol]: 316.48
CAS: 1191-65-7

Physical Properties

Property code	Value	Unit	Source
gf	293.12	kJ/mol	Joback Method
hf	-135.47	kJ/mol	Joback Method
hfus	53.94	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
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	776.97	K	Joback Method
tc	968.10	K	Joback Method
tf	373.19	K	Joback Method
vc	1.135	m3/kmol	Joback Method

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

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=C1191657&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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