Methyl 5,8,11,14-eicosatetraenoate (Methyl arachidonate)

Inchi: InChI=1S/C19H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h5-6,8-9
InchiKey: CQASFQVRWYNJFB-AFSLFLIVSA-N
Formula: C19H30O2
SMILES: CCCC=CCC=CCC=CCC=CCCCC(=O)OC
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	196.06	kJ/mol	Joback Method
hf	-211.41	kJ/mol	Joback Method
hfus	48.56	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.525		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	727.05	K	Joback Method
tc	913.66	K	Joback Method
tf	355.73	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.23	J/mol×K	727.05	Joback Method
cpg	835.84	J/mol×K	882.56	Joback Method
cpg	821.58	J/mol×K	851.46	Joback Method
cpg	806.65	J/mol×K	820.36	Joback Method
cpg	790.99	J/mol×K	789.25	Joback Method
cpg	774.54	J/mol×K	758.15	Joback Method

cpg	849.50	J/mol×K	913.66	Joback Method
dvisc	0.0000468	Pa×s	727.05	Joback Method
dvisc	0.0000634	Pa×s	665.16	Joback Method
dvisc	0.0000915	Pa×s	603.28	Joback Method
dvisc	0.0001434	Pa×s	541.39	Joback Method
dvisc	0.0002525	Pa×s	479.50	Joback Method
dvisc	0.0005256	Pa×s	417.62	Joback Method
dvisc	0.0014122	Pa×s	355.73	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R614110&Units=SI

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.