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	2217.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2216.00		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	774.54	J/mol×K	758.15	Joback Method
cpg	790.99	J/mol×K	789.25	Joback Method
cpg	806.65	J/mol×K	820.36	Joback Method
cpg	821.58	J/mol×K	851.46	Joback Method
cpg	835.84	J/mol×K	882.56	Joback Method

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

Sources

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

Latest version available from:
https://www.chemeo.com/cid/91-584-3/Methyl-5-8-11-14-eicosatetraenoate-Methyl-arachidonate.pdf
Generated by Cheméo on 2024-10-12 04:32:32.452519202 +0000 UTC m=+3288415.089488461.

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