8,11,14-Eicosatrienoic acid, methyl ester

Inchi: InChI=1S/C21H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h7
InchiKey: QHATYOWJCAQINT-SPOHZTNBSA-N
Formula: C21H36O2
SMILES: CCCCCC=CCC=CCC=CCCCCCCC(=O)OC
Mol. weight [g/mol]: 320.51
CAS: 17364-32-8

Physical Properties

Property code	Value	Unit	Source
gf	132.68	kJ/mol	Joback Method
hf	-369.91	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	71.37	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.529		Crippen Method
mcvol	301.290	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	768.65	K	Joback Method
tc	951.62	K	Joback Method
tf	383.35	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.73	J/mol×K	768.65	Joback Method
cpg	916.26	J/mol×K	799.15	Joback Method
cpg	933.90	J/mol×K	829.64	Joback Method
cpg	950.70	J/mol×K	860.14	Joback Method
cpg	966.71	J/mol×K	890.63	Joback Method
cpg	981.99	J/mol×K	921.13	Joback Method

cpg	996.60	J/mol×K	951.62	Joback Method
dvisc	0.0012267	Pa×s	383.35	Joback Method
dvisc	0.0004662	Pa×s	447.57	Joback Method
dvisc	0.0002259	Pa×s	511.78	Joback Method
dvisc	0.0001286	Pa×s	576.00	Joback Method
dvisc	0.0000820	Pa×s	640.22	Joback Method
dvisc	0.0000568	Pa×s	704.43	Joback Method
dvisc	0.0000418	Pa×s	768.65	Joback Method

Sources

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=C17364328&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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