

11,14,17-Eicosatrienoic acid, methyl ester

Other names:	Methyl 11,14,17-icosatrienoate Methyl 11,14,17-eicosatrienoate
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/h4
InchiKey:	XQAVRBUXEPJVRC-JSIPCRQOSA-N
Formula:	C21H36O2
SMILES:	CCC=CCC=CCC=CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	320.51
CAS:	55682-88-7

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	2275.00		NIST Webbook
rinpol	2241.00		NIST Webbook
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
rinpol	2290.00		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/molxK	768.65	Joback Method
cpg	916.26	J/molxK	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	Paxs	383.35	Joback Method
dvisc	0.0004662	Paxs	447.57	Joback Method
dvisc	0.0002259	Paxs	511.78	Joback Method
dvisc	0.0001286	Paxs	576.00	Joback Method
dvisc	0.0000820	Paxs	640.22	Joback Method
dvisc	0.0000568	Paxs	704.43	Joback Method
dvisc	0.0000418	Paxs	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=C55682887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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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