Cis-11,14-eicosadienoic acid, methyl ester

Other names: (all-Z)-Methyl eicosa-11,14-dienoate
11,14-Eicosadienoic acid, methyl ester, (Z,Z)
methyl Z,Z 11,14-eicosadienoate
Inchi: InChI=1S/C21H38O2/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: GWJCFAOQCNNFAM-NQLNTKRDSA-N
Formula: C21H38O2
SMILES: CCCCC/C=C\C/C=C\CCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 322.53

Physical Properties

Property code	Value	Unit	Source
af	0.8352		Cheméo Relay (1.0)
gf	52.46	kJ/mol	Joback Method
hf	-632.59	kJ/mol	Cheméo Relay (1.0)
hfus	53.34	kJ/mol	Joback Method
hvap	113.85	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-6.32		Cheméo Relay (1.0)
logp	6.753		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2305.90		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	590.85	K	Cheméo Relay (1.0)
tc	784.75	K	Cheméo Relay (1.0)
tf	259.88	K	Cheméo Relay (1.0)
vc	1.107	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.23	J/mol×K	914.06	Joback Method
cpg	1023.10	J/mol×K	943.97	Joback Method

cpg	940.85	J/mol×K	794.40	Joback Method
cpg	958.97	J/mol×K	824.32	Joback Method
cpg	976.21	J/mol×K	854.23	Joback Method
cpg	992.61	J/mol×K	884.14	Joback Method
cpg	921.82	J/mol×K	764.49	Joback Method
dvisc	0.0002544	Pa×s	513.78	Joback Method
dvisc	0.0005151	Pa×s	451.11	Joback Method
dvisc	0.0013095	Pa×s	388.43	Joback Method
dvisc	0.0001465	Pa×s	576.46	Joback Method
dvisc	0.0000940	Pa×s	639.14	Joback Method
dvisc	0.0000653	Pa×s	701.81	Joback Method
dvisc	0.0000481	Pa×s	764.49	Joback Method
hvapt	117.50	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333618&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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