cis-13,16-Docasadienoic acid, methyl ester

Other names: (Z,Z)-Methyl docosa-13,16-dienoate
methyl Z,Z 13,16-docosadienoate
Inchi: InChI=1S/C23H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)2
InchiKey: UPIRHFZFPVEDCF-NQLNTKRDSA-N
Formula: C23H42O2
SMILES: CCCCCC=CCC=CCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 350.58

Physical Properties

Property code	Value	Unit	Source
gf	69.30	kJ/mol	Joback Method
hf	-528.41	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.533		Crippen Method
mcvol	333.770	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2509.90		NIST Webbook
rinpol	2509.90		NIST Webbook
tb	810.25	K	Joback Method
tc	994.49	K	Joback Method
tf	410.97	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.92	J/mol×K	810.25	Joback Method
cpg	1063.84	J/mol×K	840.96	Joback Method
cpg	1082.76	J/mol×K	871.66	Joback Method
cpg	1100.75	J/mol×K	902.37	Joback Method
cpg	1117.85	J/mol×K	933.08	Joback Method
cpg	1134.11	J/mol×K	963.79	Joback Method

cpg	1149.58	J/mol×K	994.49	Joback Method
dvisc	0.0010459	Pa×s	410.97	Joback Method
dvisc	0.0004051	Pa×s	477.52	Joback Method
dvisc	0.0001979	Pa×s	544.06	Joback Method
dvisc	0.0001130	Pa×s	610.61	Joback Method
dvisc	0.0000721	Pa×s	677.16	Joback Method
dvisc	0.0000498	Pa×s	743.70	Joback Method
dvisc	0.0000366	Pa×s	810.25	Joback Method
hvapt	127.90	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
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
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=U333603&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
hvapt:	Enthalpy of vaporization at a given temperature
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