Methyl 11,14-eicosadienoate

Inchi: InChI=1S/C22H40O2/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: VPVGSRIJUIEFPI-MVKOLZDDSA-N
Formula: C22H40O2
SMILES: CCCCCCC=CCC=CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 336.55

Physical Properties

Property code	Value	Unit	Source
gf	60.88	kJ/mol	Joback Method
hf	-507.77	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.143		Crippen Method
mcvol	319.680	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	787.37	K	Joback Method
tc	968.88	K	Joback Method
tf	399.70	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.44	J/mol×K	787.37	Joback Method
cpg	1001.90	J/mol×K	817.62	Joback Method
cpg	1020.40	J/mol×K	847.87	Joback Method
cpg	1038.00	J/mol×K	878.13	Joback Method
cpg	1054.74	J/mol×K	908.38	Joback Method
cpg	1070.67	J/mol×K	938.63	Joback Method
cpg	1085.84	J/mol×K	968.88	Joback Method

dvisc	0.0011728	Pa×s	399.70	Joback Method
dvisc	0.0004577	Pa×s	464.31	Joback Method
dvisc	0.0002248	Pa×s	528.92	Joback Method
dvisc	0.0001289	Pa×s	593.53	Joback Method
dvisc	0.0000824	Pa×s	658.15	Joback Method
dvisc	0.0000571	Pa×s	722.76	Joback Method
dvisc	0.0000420	Pa×s	787.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R74828&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

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