Methyl 9-eicosenoate

Other names: Gadoleic acid, methyl ester
Inchi: InChI=1S/C21H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h1
InchiKey: XEJYCWVISZMIDA-SEYXRHQNSA-N
Formula: C21H40O2
SMILES: CCCCCCCCCCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]: 324.54

Physical Properties

Property code	Value	Unit	Source
gf	-27.76	kJ/mol	Joback Method
hf	-604.35	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.977		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	760.33	K	Joback Method
tc	936.69	K	Joback Method
tf	393.51	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.68	J/mol×K	760.33	Joback Method
cpg	965.24	J/mol×K	789.72	Joback Method
cpg	983.86	J/mol×K	819.12	Joback Method
cpg	1001.56	J/mol×K	848.51	Joback Method
cpg	1018.40	J/mol×K	877.90	Joback Method
cpg	1034.38	J/mol×K	907.29	Joback Method
cpg	1049.56	J/mol×K	936.69	Joback Method

dvisc	0.0013987	Pa×s	393.51	Joback Method
dvisc	0.0005689	Pa×s	454.65	Joback Method
dvisc	0.0002864	Pa×s	515.78	Joback Method
dvisc	0.0001668	Pa×s	576.92	Joback Method
dvisc	0.0001077	Pa×s	638.06	Joback Method
dvisc	0.0000751	Pa×s	699.19	Joback Method
dvisc	0.0000555	Pa×s	760.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U336505&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
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