11,14-Eicosadienoic acid, methyl ester

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-ZDVGBALWSA-N
Formula: C21H38O2
SMILES: CCCCCC=CCC=CCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 322.53
CAS: 2463-02-7

Physical Properties

Property code	Value	Unit	Source
gf	52.46	kJ/mol	Joback Method
hf	-487.13	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	71.41	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.753		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2269.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2279.00		NIST Webbook
ripol	2751.00		NIST Webbook
ripol	2725.00		NIST Webbook
tb	764.49	K	Joback Method
tc	943.97	K	Joback Method
tf	388.43	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.82	J/mol×K	764.49	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	1008.23	J/mol×K	914.06	Joback Method
cpg	1023.10	J/mol×K	943.97	Joback Method
dvisc	0.0013095	Pa×s	388.43	Joback Method
dvisc	0.0005151	Pa×s	451.11	Joback Method
dvisc	0.0002544	Pa×s	513.78	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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2463027&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume