13-Docosenoic acid, methyl ester

Other names: Methyl 13-docosenoate
Inchi: InChI=1S/C23H44O2/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: ZYNDJIBBPLNPOW-ZHACJKMWSA-N
Formula: C23H44O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 352.59
CAS: 56630-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-10.92	kJ/mol	Joback Method
hf	-645.63	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	75.91	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.757		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	806.09	K	Joback Method
tc	988.24	K	Joback Method
tf	416.05	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.83	J/mol×K	806.09	Joback Method
cpg	1089.32	J/mol×K	836.45	Joback Method
cpg	1108.77	J/mol×K	866.81	Joback Method
cpg	1127.22	J/mol×K	897.16	Joback Method
cpg	1144.72	J/mol×K	927.52	Joback Method
cpg	1161.30	J/mol×K	957.88	Joback Method

cpg	1177.00	J/mol×K	988.24	Joback Method
dvisc	0.0011170	Pa×s	416.05	Joback Method
dvisc	0.0004469	Pa×s	481.06	Joback Method
dvisc	0.0002224	Pa×s	546.06	Joback Method
dvisc	0.0001283	Pa×s	611.07	Joback Method
dvisc	0.0000823	Pa×s	676.08	Joback Method
dvisc	0.0000571	Pa×s	741.08	Joback Method
dvisc	0.0000420	Pa×s	806.09	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=C56630694&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

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