

9-Docosenoic acid, methyl ester

Other names:	22:1n-9 methyl ester
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)
InchiKey:	NVCSYLJPLYJUNW-CCEZHUSRSA-N
Formula:	C23H44O2
SMILES:	CCCCCCCCCCCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	352.59

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	2479.00		NIST Webbook
rinpol	2479.00		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/molxK	806.09	Joback Method
cpg	1089.32	J/molxK	836.45	Joback Method
cpg	1108.77	J/molxK	866.81	Joback Method
cpg	1127.22	J/molxK	897.16	Joback Method
cpg	1144.72	J/molxK	927.52	Joback Method
cpg	1161.30	J/molxK	957.88	Joback Method
cpg	1177.00	J/molxK	988.24	Joback Method

dvisc	0.0011170	Paxs	416.05	Joback Method
dvisc	0.0004469	Paxs	481.06	Joback Method
dvisc	0.0002224	Paxs	546.06	Joback Method
dvisc	0.0001283	Paxs	611.07	Joback Method
dvisc	0.0000823	Paxs	676.08	Joback Method
dvisc	0.0000571	Paxs	741.08	Joback Method
dvisc	0.0000420	Paxs	806.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R99393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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