

7,10,13,16-Docosatetraenoic acid, methyl ester

Inchi:	InChI=1S/C23H38O2/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:	ABGHYAFHPINIHF-SHDWVJIKSA-N
Formula:	C23H38O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCCCCC(=O)OC
Mol. weight [g/mol]:	346.55

Physical Properties

Property code	Value	Unit	Source
gf	229.74	kJ/mol	Joback Method
hf	-293.97	kJ/mol	Joback Method
hfus	58.92	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	7.085		Crippen Method
mcvol	325.170	ml/mol	McGowan Method
pc	993.88	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	818.57	K	Joback Method
tc	1008.12	K	Joback Method
tf	400.81	K	Joback Method
vc	1.268	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.49	J/molxK	818.57	Joback Method
cpg	1012.37	J/molxK	850.16	Joback Method
cpg	1030.36	J/molxK	881.75	Joback Method
cpg	1047.54	J/molxK	913.35	Joback Method
cpg	1063.99	J/molxK	944.94	Joback Method
cpg	1079.77	J/molxK	976.53	Joback Method
cpg	1094.97	J/molxK	1008.12	Joback Method
dvisc	0.0009188	Paxs	400.81	Joback Method

dvisc	0.0003329	Paxs	470.44	Joback Method
dvisc	0.0001567	Paxs	540.06	Joback Method
dvisc	0.0000876	Paxs	609.69	Joback Method
dvisc	0.0000552	Paxs	679.32	Joback Method
dvisc	0.0000379	Paxs	748.94	Joback Method
dvisc	0.0000277	Paxs	818.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R98793&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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