

10,13-Docosadienoic acid, methyl ester

Inchi:	InChI=1S/C23H42O2/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:	QXCRCRVQJUAXGL-IWCZYTNSA-N
Formula:	C23H42O2
SMILES:	CCCCCCCC=CCC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	350.58

Physical Properties

Property code	Value	Unit	Source
gf	69.30	kJ/mol	Joback Method
hf	-528.41	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.533		Crippen Method
mvol	333.770	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	810.25	K	Joback Method
tc	994.49	K	Joback Method
tf	410.97	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.92	J/molxK	810.25	Joback Method
cpg	1134.11	J/molxK	963.79	Joback Method
cpg	1117.85	J/molxK	933.08	Joback Method
cpg	1100.75	J/molxK	902.37	Joback Method
cpg	1082.76	J/molxK	871.66	Joback Method
cpg	1063.84	J/molxK	840.96	Joback Method
cpg	1149.58	J/molxK	994.49	Joback Method
dvisc	0.0000366	Paxs	810.25	Joback Method

dvisc	0.0000498	Paxs	743.70	Joback Method
dvisc	0.0000721	Paxs	677.16	Joback Method
dvisc	0.0001130	Paxs	610.61	Joback Method
dvisc	0.0001979	Paxs	544.06	Joback Method
dvisc	0.0004051	Paxs	477.52	Joback Method
dvisc	0.0010459	Paxs	410.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R98832&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

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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