

11,13-Eicosadienoic acid, methyl ester

Other names:	Methyl 11,13-icosadienoate Methyl 11,13-eicosadienoate
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/h8
InchiKey:	QKVKDCGPQOJFNM-BNFZFUHLSA-N
Formula:	C21H38O2
SMILES:	CCCCCCC=CC=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	322.53
CAS:	56599-57-6

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
mvol	305.590	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
ripol	2583.00		NIST Webbook
ripol	2583.00		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/molxK	764.49	Joback Method
cpg	1008.23	J/molxK	914.06	Joback Method
cpg	992.61	J/molxK	884.14	Joback Method
cpg	976.21	J/molxK	854.23	Joback Method
cpg	958.97	J/molxK	824.32	Joback Method

cpg	940.85	J/molxK	794.40	Joback Method
cpg	1023.10	J/molxK	943.97	Joback Method
dvisc	0.0000481	Paxs	764.49	Joback Method
dvisc	0.0000653	Paxs	701.81	Joback Method
dvisc	0.0000940	Paxs	639.14	Joback Method
dvisc	0.0001465	Paxs	576.46	Joback Method
dvisc	0.0002544	Paxs	513.78	Joback Method
dvisc	0.0005151	Paxs	451.11	Joback Method
dvisc	0.0013095	Paxs	388.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56599576&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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