

isopropyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate

Other names:	isopropyllinolenate
Inchi:	InChI=1S/C21H36O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20(2)3/h5
InchiKey:	SQOVKJOWVZUDDC-AGRJPVHOSA-N
Formula:	C21H36O2
SMILES:	CCC=CCC=CCC=CCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]:	320.51
CAS:	83918-59-6

Physical Properties

Property code	Value	Unit	Source
gf	130.24	kJ/mol	Joback Method
hf	-375.19	kJ/mol	Joback Method
hfus	50.02	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.527		Crippen Method
mcvol	301.290	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2200.30		NIST Webbook
rinpol	2200.30		NIST Webbook
tb	768.21	K	Joback Method
tc	952.78	K	Joback Method
tf	368.35	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.21	J/molxK	768.21	Joback Method
cpg	983.10	J/molxK	922.02	Joback Method
cpg	967.73	J/molxK	891.26	Joback Method
cpg	951.62	J/molxK	860.50	Joback Method
cpg	934.69	J/molxK	829.73	Joback Method
cpg	916.91	J/molxK	798.97	Joback Method

cpg	997.76	J/mol×K	952.78	Joback Method
dvisc	0.0000385	Paxs	768.21	Joback Method
dvisc	0.0000532	Paxs	701.57	Joback Method
dvisc	0.0000787	Paxs	634.92	Joback Method
dvisc	0.0001278	Paxs	568.28	Joback Method
dvisc	0.0002359	Paxs	501.64	Joback Method
dvisc	0.0005256	Paxs	434.99	Joback Method
dvisc	0.0015646	Paxs	368.35	Joback Method

Sources

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=C83918596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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