

Isopropyl linoleate

Other names:	9,12-Octadecadienoic acid (Z,Z)-, 1-methylethyl ester Ceraphyl IPL isopropyl (9Z,12Z)-octadeca-9,12-dienoate
Inchi:	InChI=1S/C21H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20(2)3/h8
InchiKey:	XEIOPEQGDSYOIH-MURFETPASA-N
Formula:	C21H38O2
SMILES:	CCCCC=CCC=CCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]:	322.53
CAS:	22882-95-7

Physical Properties

Property code	Value	Unit	Source
gf	50.02	kJ/mol	Joback Method
hf	-492.41	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.752		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
tb	764.05	K	Joback Method
tc	944.91	K	Joback Method
tf	373.43	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.28	J/molxK	764.05	Joback Method
cpg	1009.26	J/molxK	914.76	Joback Method
cpg	993.57	J/molxK	884.62	Joback Method
cpg	977.08	J/molxK	854.48	Joback Method
cpg	959.72	J/molxK	824.34	Joback Method
cpg	941.47	J/molxK	794.19	Joback Method

cpg	1024.19	J/mol×K	944.91	Joback Method
dvisc	0.0000443	Paxs	764.05	Joback Method
dvisc	0.0000612	Paxs	698.95	Joback Method
dvisc	0.0000903	Paxs	633.84	Joback Method
dvisc	0.0001456	Paxs	568.74	Joback Method
dvisc	0.0002657	Paxs	503.64	Joback Method
dvisc	0.0005796	Paxs	438.53	Joback Method
dvisc	0.0016597	Paxs	373.43	Joback Method

Sources

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=C22882957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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