i-Propyl 9-octadecenoate

Other names: Octadecenoic acid, 1-methylethyl ester
Inchi: InChI=1S/C21H40O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20(2)3/h1
InchiKey: PZQSQRCNMZGWFT-QXMHVHEDSA-N
Formula: C21H40O2
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]: 324.54

Physical Properties

Property code	Value	Unit	Source
gf	-30.20	kJ/mol	Joback Method
hf	-609.63	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	71.07	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.976		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2192.00		NIST Webbook
tb	759.89	K	Joback Method
tc	937.41	K	Joback Method
tf	378.51	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.13	J/mol×K	759.89	Joback Method
cpg	965.83	J/mol×K	789.48	Joback Method
cpg	984.57	J/mol×K	819.06	Joback Method
cpg	1002.38	J/mol×K	848.65	Joback Method
cpg	1019.29	J/mol×K	878.24	Joback Method
cpg	1035.34	J/mol×K	907.82	Joback Method
cpg	1050.57	J/mol×K	937.41	Joback Method
dvisc	0.0017622	Pa×s	378.51	Joback Method

dvisc	0.0006391	Pa×s	442.07	Joback Method
dvisc	0.0002991	Pa×s	505.64	Joback Method
dvisc	0.0001658	Pa×s	569.20	Joback Method
dvisc	0.0001035	Pa×s	632.76	Joback Method
dvisc	0.0000704	Pa×s	696.33	Joback Method
dvisc	0.0000511	Pa×s	759.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U336671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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