i-Propyl 9-hexadecenoate

Other names: Hexadecenoic acid, 1-methylethyl ester
Inchi: InChI=1S/C19H36O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18(2)3/h9-10,18
InchiKey: VGLJNQYCGDBABV-KTKRTIGZSA-N
Formula: C19H36O2
SMILES: CCCCCCC=CCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-47.04	kJ/mol	Joback Method
hf	-568.35	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.195		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	714.13	K	Joback Method
tc	889.04	K	Joback Method
tf	355.97	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.63	J/mol×K	714.13	Joback Method
cpg	845.57	J/mol×K	743.28	Joback Method
cpg	863.61	J/mol×K	772.43	Joback Method
cpg	880.78	J/mol×K	801.59	Joback Method
cpg	897.13	J/mol×K	830.74	Joback Method
cpg	912.66	J/mol×K	859.89	Joback Method
cpg	927.42	J/mol×K	889.04	Joback Method

dvisc	0.0022073	Pa×s	355.97	Joback Method
dvisc	0.0008110	Pa×s	415.66	Joback Method
dvisc	0.0003832	Pa×s	475.36	Joback Method
dvisc	0.0002140	Pa×s	535.05	Joback Method
dvisc	0.0001344	Pa×s	594.74	Joback Method
dvisc	0.0000918	Pa×s	654.44	Joback Method
dvisc	0.0000669	Pa×s	714.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U336628&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