Nonanoic acid, undecyl ester

Inchi: InChI=1S/C20H40O2/c1-3-5-7-9-11-12-13-15-17-19-22-20(21)18-16-14-10-8-6-4-2/h3-19
InchiKey: CNLZXBFSQDBMHB-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCC
Mol. weight [g/mol]: 312.53

Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	387.32	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
dvisc	0.0000733	Pa×s	733.29	Joback Method

dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0002156	Pa×s	560.30	Joback Method
dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0007053	Pa×s	444.98	Joback Method
dvisc	0.0016619	Pa×s	387.32	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=U340278&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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