NONANOIC ACID, OCTYL ESTER

Other names: octyl nonanoate
Inchi: InChI=1S/C17H34O2/c1-3-5-7-9-11-13-15-17(18)19-16-14-12-10-8-6-4-2/h3-16H2,1-2H3
InchiKey: XMCQOINBECWLBL-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCCCCCCOC(=O)CCCCCCCC
Mol. weight [g/mol]: 270.46

Physical Properties

Property code	Value	Unit	Source
af	0.8704		Cheméo Relay (1.0)
hf	-710.76	kJ/mol	Cheméo Relay (1.0)
hfus	42.57	kJ/mol	Joback Method
hvap	83.73	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-5.77		Cheméo Relay (1.0)
logp	5.641		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	571.13	K	Cheméo Relay (1.0)
tc	749.98	K	Cheméo Relay (1.0)
tf	270.01	K	Cheméo Relay (1.0)
vc	1.011	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.28	J/mol×K	664.65	Joback Method
cpg	750.62	J/mol×K	692.59	Joback Method
cpg	768.17	J/mol×K	720.52	Joback Method
cpg	784.95	J/mol×K	748.46	Joback Method
cpg	800.97	J/mol×K	776.39	Joback Method
cpg	816.25	J/mol×K	804.33	Joback Method

cpg	830.80	J/mol×K	832.26	Joback Method
dvisc	0.0022120	Pa×s	353.51	Joback Method
dvisc	0.0009695	Pa×s	405.37	Joback Method
dvisc	0.0005124	Pa×s	457.22	Joback Method
dvisc	0.0003083	Pa×s	509.08	Joback Method
dvisc	0.0002038	Pa×s	560.94	Joback Method
dvisc	0.0001445	Pa×s	612.79	Joback Method
dvisc	0.0001081	Pa×s	664.65	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5303264&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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