3-Octenoic acid, nonyl ester

Inchi: InChI=1S/C17H32O2/c1-3-5-7-9-10-12-14-16-19-17(18)15-13-11-8-6-4-2/h11,13H,3-10,1
InchiKey: RSDRNZAHWSORFS-ACCUITESSA-N
Formula: C17H32O2
SMILES: CCCCC=CCC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-61.44	kJ/mol	Joback Method
hf	-521.79	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	668.81	K	Joback Method
tc	841.03	K	Joback Method
tf	348.43	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/mol×K	668.81	Joback Method
cpg	728.86	J/mol×K	697.51	Joback Method
cpg	745.96	J/mol×K	726.22	Joback Method
cpg	762.28	J/mol×K	754.92	Joback Method
cpg	777.84	J/mol×K	783.62	Joback Method
cpg	792.67	J/mol×K	812.33	Joback Method
cpg	806.79	J/mol×K	841.03	Joback Method
dvisc	0.0020673	Pa×s	348.43	Joback Method

dvisc	0.0008745	Pa×s	401.83	Joback Method
dvisc	0.0004527	Pa×s	455.22	Joback Method
dvisc	0.0002691	Pa×s	508.62	Joback Method
dvisc	0.0001766	Pa×s	562.02	Joback Method
dvisc	0.0001246	Pa×s	615.41	Joback Method
dvisc	0.0000930	Pa×s	668.81	Joback Method

Sources

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=U406129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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