

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
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tb	668.81	K	Joback Method
tc	841.03	K	Joback Method
tf	348.43	K	Joback Method
vc	0.992	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0008745	Paxs	401.83	Joback Method
dvisc	0.0004527	Paxs	455.22	Joback Method
dvisc	0.0002691	Paxs	508.62	Joback Method
dvisc	0.0001766	Paxs	562.02	Joback Method
dvisc	0.0001246	Paxs	615.41	Joback Method
dvisc	0.0000930	Paxs	668.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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