

2-Heptenoic acid, nonyl ester

Inchi:	InChI=1S/C16H30O2/c1-3-5-7-9-10-11-13-15-18-16(17)14-12-8-6-4-2/h12,14H,3-11,13,15H
InchiKey:	RVUUGRKPBSTXDB-WYMLVPIESA-N
Formula:	C16H30O2
SMILES:	CCCCC=CC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
gf	-69.86	kJ/mol	Joback Method
hf	-501.15	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.027		Crippen Method
mvol	239.440	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	645.93	K	Joback Method
tc	818.34	K	Joback Method
tf	337.16	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.12	J/molxK	645.93	Joback Method
cpg	672.59	J/molxK	674.67	Joback Method
cpg	689.29	J/molxK	703.40	Joback Method
cpg	705.23	J/molxK	732.14	Joback Method
cpg	720.44	J/molxK	760.87	Joback Method
cpg	734.94	J/molxK	789.61	Joback Method
cpg	748.76	J/molxK	818.34	Joback Method
dvisc	0.0022449	Paxs	337.16	Joback Method

dvisc	0.0009605	Paxs	388.62	Joback Method
dvisc	0.0005012	Paxs	440.08	Joback Method
dvisc	0.0002997	Paxs	491.55	Joback Method
dvisc	0.0001976	Paxs	543.01	Joback Method
dvisc	0.0001400	Paxs	594.47	Joback Method
dvisc	0.0001048	Paxs	645.93	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=U406095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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