

NONANE, 1,1-DIMETHOXY-

Other names:	Nonane, 1,1-dimethoxy- n-Nonanal dimethyl acetal 1,1-dimethoxynonane
Inchi:	InChI=1S/C11H24O2/c1-4-5-6-7-8-9-10-11(12-2)13-3/h11H,4-10H2,1-3H3
InchiKey:	LYLVOCPDQAOQKL-UHFFFAOYSA-N
Formula:	C11H24O2
SMILES:	CCCCCCCCC(OC)OC
Mol. weight [g/mol]:	188.31

Physical Properties

Property code	Value	Unit	Source
af	0.5713		Cheméo Relay (1.0)
gf	-170.70	kJ/mol	Joback Method
hf	-531.58	kJ/mol	Cheméo Relay (1.0)
hfus	23.10	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.356		Crippen Method
mcvol	177.590	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1267.00		NIST Webbook
rinpol	1267.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1465.00		NIST Webbook
tb	484.55	K	Cheméo Relay (1.0)
tc	646.17	K	Cheméo Relay (1.0)
tf	224.55	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.01	J/mol×K	495.48	Joback Method

cpg	431.77	J/mol×K	522.96	Joback Method
cpg	447.02	J/mol×K	550.45	Joback Method
cpg	461.75	J/mol×K	577.93	Joback Method
cpg	475.97	J/mol×K	605.41	Joback Method
cpg	489.68	J/mol×K	632.90	Joback Method
cpg	502.88	J/mol×K	660.38	Joback Method
dvisc	0.0044998	Pa×s	243.19	Joback Method
dvisc	0.0016771	Pa×s	285.24	Joback Method
dvisc	0.0008055	Pa×s	327.29	Joback Method
dvisc	0.0004572	Pa×s	369.34	Joback Method
dvisc	0.0002913	Pa×s	411.38	Joback Method
dvisc	0.0002018	Pa×s	453.43	Joback Method
dvisc	0.0001488	Pa×s	495.48	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18824630&Units=SI>

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

Legend

af:	Acentric Factor
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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<https://www.chemeo.com/cid/81-184-8/NONANE-1-1-DIMETHOXY.pdf>

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