

2-Nonene, 4,6-dimethyl, # 1

Inchi:	InChI=1S/C11H22/c1-5-7-10(3)9-11(4)8-6-2/h5,7,10-11H,6,8-9H2,1-4H3/b7-5+
InchiKey:	ONGPAIHWJMXYLD-FNORWQNLSA-N
Formula:	C11H22
SMILES:	CC=CC(C)CC(C)CCC
Mol. weight [g/mol]:	154.29

Physical Properties

Property code	Value	Unit	Source
gf	117.08	kJ/mol	Joback Method
hf	-163.71	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	39.26	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	4.025		Crippen Method
mcvol	161.550	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	998.00		NIST Webbook
rinpol	998.00		NIST Webbook
tb	454.36	K	Joback Method
tc	630.87	K	Joback Method
tf	178.65	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.70	J/mol×K	454.36	Joback Method
cpg	420.97	J/mol×K	601.45	Joback Method
cpg	407.08	J/mol×K	572.03	Joback Method
cpg	392.54	J/mol×K	542.62	Joback Method
cpg	377.31	J/mol×K	513.20	Joback Method
cpg	361.37	J/mol×K	483.78	Joback Method
cpg	434.23	J/mol×K	630.87	Joback Method
dvisc	0.0001718	Pa×s	454.36	Joback Method

dvisc	0.0002429	Pa×s	408.41	Joback Method
dvisc	0.0003749	Pa×s	362.46	Joback Method
dvisc	0.0006563	Pa×s	316.50	Joback Method
dvisc	0.0013897	Pa×s	270.55	Joback Method
dvisc	0.0040002	Pa×s	224.60	Joback Method
dvisc	0.0198348	Pa×s	178.65	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=R568319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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