

2-Methyl-1-nonene

Other names:	1-Nonene, 2-methyl-
Inchi:	InChI=1S/C10H20/c1-4-5-6-7-8-9-10(2)3/h2,4-9H2,1,3H3
InchiKey:	YLZQHQUVNZVGOK-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	C=C(C)CCCCCCC
Mol. weight [g/mol]:	140.27
CAS:	2980-71-4

Physical Properties

Property code	Value	Unit	Source
gf	112.61	kJ/mol	Joback Method
hf	-134.09	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	978.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	424.76	K	Joback Method
tc	593.45	K	Joback Method
tf	186.74	K	Joback Method
vc	0.578	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.06	J/mol×K	424.76	Joback Method
cpg	313.92	J/mol×K	452.88	Joback Method
cpg	328.19	J/mol×K	480.99	Joback Method
cpg	341.88	J/mol×K	509.11	Joback Method
cpg	355.03	J/mol×K	537.22	Joback Method
cpg	367.63	J/mol×K	565.34	Joback Method
cpg	379.71	J/mol×K	593.45	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol345.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2980714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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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