

(E) 1-Methyl-1-cyclooctene

Inchi:	InChI=1S/C9H16/c1-9-7-5-3-2-4-6-8-9/h7H,2-6,8H2,1H3/b9-7+
InchiKey:	WFLPGXDWMZEHGP-VQHVLOKHSA-N
Formula:	C9H16
SMILES:	CC1=CCCCCCC1
Mol. weight [g/mol]:	124.22
CAS:	38229-26-4

Physical Properties

Property code	Value	Unit	Source
gf	53.19	kJ/mol	Joback Method
hf	-5.40	kJ/mol	NIST Webbook
hfus	6.46	kJ/mol	Joback Method
hvap	37.66	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	442.22	K	Joback Method
tc	662.12	K	Joback Method
tf	209.05	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.52	J/molxK	442.22	Joback Method
cpg	325.80	J/molxK	625.47	Joback Method
cpg	310.77	J/molxK	588.82	Joback Method
cpg	294.85	J/molxK	552.17	Joback Method
cpg	278.01	J/molxK	515.52	Joback Method
cpg	260.24	J/molxK	478.87	Joback Method
cpg	339.93	J/molxK	662.12	Joback Method
dvisc	0.0001869	Paxs	442.22	Joback Method
dvisc	0.0002772	Paxs	403.36	Joback Method

dvisc	0.0004473	Paxs	364.50	Joback Method
dvisc	0.0008089	Paxs	325.63	Joback Method
dvisc	0.0017176	Paxs	286.77	Joback Method
dvisc	0.0046185	Paxs	247.91	Joback Method
dvisc	0.0179390	Paxs	209.05	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=C38229264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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