OCTANE, 1-METHOXY-

Other names:	n-Octyl methyl ether
	Ether, methyl octyl
	Octyl methyl ether
	Methyl octyl ether
	1-Methoxyoctane
Inchi:	InChI=1S/C9H20O/c1-3-4-5-6-7-8-9-10-2/h3-9H2,1-2H3
InchiKey:	RIAWWRJHTAZJSU-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCCCCCOC
Mol. weight [g/mol]:	144.26

Physical Properties

Property code	Value	Unit	Source
af	0.5065		Cheméo Relay (1.0)
gf	-80.10	kJ/mol	Joback Method
hf	-348.62	kJ/mol	Cheméo Relay (1.0)
hfus	20.25	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.993		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1029.50		NIST Webbook
rinpol	1026.30		NIST Webbook
rinpol	1026.30		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1024.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1152.00		NIST Webbook
tb	445.20 ± 0.80	K	NIST Webbook
tc	609.14	K	Cheméo Relay (1.0)
tf	220.70 ± 0.80	K	NIST Webbook
tf	216.70 ± 0.50	K	NIST Webbook
vc	0.556	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.84	J/mol×K	427.74	Joback Method
cpg	312.62	J/mol×K	454.96	Joback Method
cpg	325.97	J/mol×K	482.19	Joback Method
cpg	338.88	J/mol×K	509.41	Joback Method
cpg	351.35	J/mol×K	536.63	Joback Method
cpg	363.40	J/mol×K	563.86	Joback Method
cpg	375.02	J/mol×K	591.08	Joback Method
dvisc	0.0042964	Pa×s	213.42	Joback Method
dvisc	0.0018183	Pa×s	249.14	Joback Method
dvisc	0.0009547	Pa×s	284.86	Joback Method
dvisc	0.0005787	Pa×s	320.58	Joback Method
dvisc	0.0003878	Pa×s	356.30	Joback Method
dvisc	0.0002795	Pa×s	392.02	Joback Method
dvisc	0.0002128	Pa×s	427.74	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C929566&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