

1-Octen-3-ol, methyl ether

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H18O/c1-4-6-7-8-9(5-2)10-3/h5,9H,2,4,6-8H2,1,3H3

GHUUIEXEEIVCRY-UHFFFAOYSA-N

C9H18O

C=CC(CCCCC)OC

142.24

Physical Properties

Property code	Value	Unit	Source
gf	5.30	kJ/mol	Joback Method
hf	-241.16	kJ/mol	Joback Method
hfus	15.45	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.768		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	946.10		NIST Webbook
rinpol	946.10		NIST Webbook
tb	423.98	K	Joback Method
tc	594.17	K	Joback Method
tf	196.66	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.84	J/mol×K	423.98	Joback Method
cpg	296.49	J/mol×K	452.34	Joback Method
cpg	309.65	J/mol×K	480.71	Joback Method
cpg	322.33	J/mol×K	509.07	Joback Method
cpg	334.55	J/mol×K	537.44	Joback Method
cpg	346.30	J/mol×K	565.80	Joback Method
cpg	357.59	J/mol×K	594.17	Joback Method
dvisc	0.0061645	Pa×s	196.66	Joback Method

dvisc	0.0022032	Pa×s	234.55	Joback Method
dvisc	0.0010483	Pa×s	272.43	Joback Method
dvisc	0.0005980	Pa×s	310.32	Joback Method
dvisc	0.0003855	Pa×s	348.21	Joback Method
dvisc	0.0002708	Pa×s	386.09	Joback Method
dvisc	0.0002027	Pa×s	423.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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