Octane, 1-(1-methoxyethoxy)-

Other names: Ethanal, methyl octyl acetal
Inchi: InChI=1S/C11H24O2/c1-4-5-6-7-8-9-10-13-11(2)12-3/h11H,4-10H2,1-3H3
InchiKey: RGHNITKXFLTYCG-UHFFFAOYSA-N
Formula: C11H24O2
SMILES: CCCCCCCCOC(C)OC
Mol. weight [g/mol]: 188.31
CAS: 54789-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-170.70	kJ/mol	Joback Method
hf	-540.09	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.356		Crippen Method
mcvol	177.590	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	495.48	K	Joback Method
tc	660.38	K	Joback Method
tf	243.19	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.01	J/mol×K	495.48	Joback Method
cpg	431.77	J/mol×K	522.96	Joback Method
cpg	447.02	J/mol×K	550.45	Joback Method
cpg	461.75	J/mol×K	577.93	Joback Method

cpg	475.97	J/mol×K	605.41	Joback Method
cpg	489.68	J/mol×K	632.90	Joback Method
cpg	502.88	J/mol×K	660.38	Joback Method
dvisc	0.0044998	Pa×s	243.19	Joback Method
dvisc	0.0016771	Pa×s	285.24	Joback Method
dvisc	0.0008055	Pa×s	327.29	Joback Method
dvisc	0.0004572	Pa×s	369.34	Joback Method
dvisc	0.0002913	Pa×s	411.38	Joback Method
dvisc	0.0002018	Pa×s	453.43	Joback Method
dvisc	0.0001488	Pa×s	495.48	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54789263&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

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