

Octane, 1-ethoxy-

Other names:	1-ethoxyoctane 3-oxaundecane ether, ethyl octyl ethyl octyl ether octyl ethyl ether
Inchi:	InChI=1S/C10H22O/c1-3-5-6-7-8-9-10-11-4-2/h3-10H2,1-2H3
InchiKey:	WJVJBXHEMGMVIMM-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCCCCOCC
Mol. weight [g/mol]:	158.28
CAS:	929-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-71.68	kJ/mol	Joback Method
hf	-381.95	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.383		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1084.00		NIST Webbook
tb	459.70 ± 0.80	K	NIST Webbook
tc	613.22	K	Joback Method
tf	222.20 ± 0.80	K	NIST Webbook
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.40	J/mol×K	450.62	Joback Method
cpg	357.17	J/mol×K	477.72	Joback Method
cpg	371.45	J/mol×K	504.82	Joback Method

cpg	385.25	J/mol×K	531.92	Joback Method
cpg	398.57	J/mol×K	559.02	Joback Method
cpg	411.42	J/mol×K	586.12	Joback Method
cpg	423.80	J/mol×K	613.22	Joback Method
dvisc	0.0043485	Paxs	224.69	Joback Method
dvisc	0.0018076	Paxs	262.35	Joback Method
dvisc	0.0009367	Paxs	300.00	Joback Method
dvisc	0.0005620	Paxs	337.65	Joback Method
dvisc	0.0003736	Paxs	375.31	Joback Method
dvisc	0.0002676	Paxs	412.97	Joback Method
dvisc	0.0002026	Paxs	450.62	Joback Method

Sources

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=C929613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental Study of Chemical Equilibria in the Liquid-Phase Reaction between 1-Octanol and Ethanol to 1-Ethoxyoctane:	https://www.doi.org/10.1021/je400291y

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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