

Octane, 1-propoxy-

Other names:	Ether, octyl propyl n-Octyl propyl ether 1-Propoxyoctane Octyl propyl ether Propyl octyl ether
Inchi:	InChI=1S/C11H24O/c1-3-5-6-7-8-9-11-12-10-4-2/h3-11H2,1-2H3
InchiKey:	KPFDWNLAMXJSNJ-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCCCCCCCOCCC
Mol. weight [g/mol]:	172.31
CAS:	29379-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-63.26	kJ/mol	Joback Method
hf	-402.59	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	58.80 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.51		Crippen Method
logp	3.773		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
tb	477.20 ± 1.00	K	NIST Webbook
tc	635.31	K	Joback Method
tf	227.20 ± 0.80	K	NIST Webbook
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.04	J/mol×K	473.50	Joback Method
cpg	461.04	J/mol×K	608.34	Joback Method
cpg	447.47	J/mol×K	581.37	Joback Method
cpg	433.40	J/mol×K	554.41	Joback Method

cpg	418.81	J/mol×K	527.44	Joback Method
cpg	403.69	J/mol×K	500.47	Joback Method
cpg	474.10	J/mol×K	635.31	Joback Method
dvisc	0.0001903	Pa×s	473.50	Joback Method
dvisc	0.0002526	Pa×s	433.91	Joback Method
dvisc	0.0003548	Pa×s	394.32	Joback Method
dvisc	0.0005375	Pa×s	354.73	Joback Method
dvisc	0.0009041	Pa×s	315.14	Joback Method
dvisc	0.0017659	Pa×s	275.55	Joback Method
dvisc	0.0043175	Pa×s	235.96	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=C29379417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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