Propyl tert-octyl ether

Other names: pentane, 2-propoxy-2,4,4-trimethyl-
propyl 1,1,3,3-tetramethylbutyl ether
Inchi: InChI=1S/C11H24O/c1-7-8-12-11(5,6)9-10(2,3)4/h7-9H2,1-6H3
InchiKey: LAAOKLJBELVTBX-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CCCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]: 172.31

Physical Properties

Property code	Value	Unit	Source
gf	-57.58	kJ/mol	Joback Method
hf	-420.09	kJ/mol	Joback Method
hfus	10.61	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.628		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1027.00		NIST Webbook
tb	467.04	K	Joback Method
tc	648.59	K	Joback Method
tf	240.80	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.33	J/mol×K	648.59	Joback Method
cpg	410.80	J/mol×K	497.30	Joback Method
cpg	428.19	J/mol×K	527.56	Joback Method
cpg	444.70	J/mol×K	557.81	Joback Method
cpg	460.37	J/mol×K	588.07	Joback Method
cpg	475.24	J/mol×K	618.33	Joback Method
cpg	392.51	J/mol×K	467.04	Joback Method

dvisc	0.0002760	Pa×s	429.33	Joback Method
dvisc	0.0004273	Pa×s	391.63	Joback Method
dvisc	0.0007262	Pa×s	353.92	Joback Method
dvisc	0.0014004	Pa×s	316.21	Joback Method
dvisc	0.0032266	Pa×s	278.51	Joback Method
dvisc	0.0001913	Pa×s	467.04	Joback Method
dvisc	0.0096548	Pa×s	240.80	Joback Method
pvap	0.14	kPa	292.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.16	kPa	294.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.19	kPa	296.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.20	kPa	297.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.12	kPa	289.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.22	kPa	298.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.23	kPa	299.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.24	kPa	300.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.26	kPa	301.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.28	kPa	302.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.30	kPa	303.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.32	kPa	304.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.33	kPa	305.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.36	kPa	306.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.38	kPa	307.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.39	kPa	308.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.09	kPa	286.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.07	kPa	283.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.06	kPa	280.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.05	kPa	278.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.04	kPa	277.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.03	kPa	274.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	0.21	kPa	297.80	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	

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=R559850&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers:	https://www.doi.org/10.1021/je0255980

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume