Hexyl tert-octyl ether

Other names: pentane, 2-hexoxy-2,4,4-trimethyl-
Inchi: InChI=1S/C14H30O/c1-7-8-9-10-11-15-14(5,6)12-13(2,3)4/h7-12H2,1-6H3
InchiKey: IQAABZUKUXMNOI-UHFFFAOYSA-N
Formula: C14H30O
SMILES: CCCCCCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]: 214.39

Physical Properties

Property code	Value	Unit	Source
gf	-32.32	kJ/mol	Joback Method
hf	-482.01	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.798		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
tb	535.68	K	Joback Method
tc	712.21	K	Joback Method
tf	274.61	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.20	J/mol×K	565.10	Joback Method
cpg	580.13	J/mol×K	594.52	Joback Method
cpg	598.14	J/mol×K	623.94	Joback Method
cpg	615.26	J/mol×K	653.37	Joback Method
cpg	631.53	J/mol×K	682.79	Joback Method
cpg	646.99	J/mol×K	712.21	Joback Method
cpg	541.30	J/mol×K	535.68	Joback Method

dvisc	0.0022463	Pa×s	318.12	Joback Method
dvisc	0.0009657	Pa×s	361.63	Joback Method
dvisc	0.0004977	Pa×s	405.14	Joback Method
dvisc	0.0002917	Pa×s	448.66	Joback Method
dvisc	0.0001879	Pa×s	492.17	Joback Method
dvisc	0.0068272	Pa×s	274.61	Joback Method
dvisc	0.0001300	Pa×s	535.68	Joback Method
pvap	0.05	kPa	326.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.04	kPa	323.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	320.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	320.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	317.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	314.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	311.00	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.01	kPa	308.00	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.01	kPa	304.90	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	8.60e-03	kPa	301.90	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	6.90e-03	kPa	298.80	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	5.30e-03	kPa	295.80	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559741&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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume