

Ethyl tert-octyl ether

Other names:	ethyl 1,1,3,3-tetramethylbutyl ether pentane, 2-ethoxy-2,4,4-trimethyl-
Inchi:	InChI=1S/C10H22O/c1-7-11-10(5,6)8-9(2,3)4/h7-8H2,1-6H3
InchiKey:	JGPJRBWLBUGAQN-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	158.28

Physical Properties

Property code	Value	Unit	Source
gf	-66.00	kJ/mol	Joback Method
hf	-399.45	kJ/mol	Joback Method
hfus	8.02	kJ/mol	Joback Method
hvap	37.67	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	3.238		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
tb	444.16	K	Joback Method
tc	627.37	K	Joback Method
tf	229.53	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.31	J/molxK	627.37	Joback Method
cpg	364.02	J/molxK	474.69	Joback Method
cpg	380.71	J/molxK	505.23	Joback Method
cpg	396.55	J/molxK	535.76	Joback Method
cpg	411.57	J/molxK	566.30	Joback Method
cpg	425.81	J/molxK	596.83	Joback Method

cpg	346.46	J/molxK	444.16	Joback Method
dvisc	0.0106846	Paxs	229.53	Joback Method
dvisc	0.0035930	Paxs	265.30	Joback Method
dvisc	0.0015654	Paxs	301.07	Joback Method
dvisc	0.0008136	Paxs	336.84	Joback Method
dvisc	0.0004795	Paxs	372.62	Joback Method
dvisc	0.0002150	Paxs	444.16	Joback Method
dvisc	0.0003100	Paxs	408.39	Joback Method
pvap	0.09	kPa	274.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.12	kPa	277.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.14	kPa	280.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.18	kPa	283.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.22	kPa	286.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.28	kPa	289.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.34	kPa	292.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.41	kPa	295.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.51	kPa	298.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.60	kPa	301.20	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=R559692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Infinite dilution activity coefficient measurements by inert gas stripping method:	https://www.doi.org/10.1016/j.fluid.2006.02.022
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

cp_g:	Ideal gas heat capacity
d_{visc}:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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

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