

Pentyl tert-octyl ether

Other names:	pentane, 2-pentoxy-2,4,4-trimethyl-
Inchi:	InChI=1S/C13H28O/c1-7-8-9-10-14-13(5,6)11-12(2,3)4/h7-11H2,1-6H3
InchiKey:	ZNFVRHLUNVCECG-UHFFFAOYSA-N
Formula:	C13H28O
SMILES:	CCCCCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	200.36

Physical Properties

Property code	Value	Unit	Source
gf	-40.74	kJ/mol	Joback Method
hf	-461.37	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.408		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	512.80	K	Joback Method
tc	690.95	K	Joback Method
tf	263.34	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.22	J/mol×K	690.95	Joback Method
cpg	509.48	J/mol×K	542.49	Joback Method
cpg	527.97	J/mol×K	572.18	Joback Method
cpg	545.56	J/mol×K	601.87	Joback Method
cpg	562.27	J/mol×K	631.57	Joback Method
cpg	578.15	J/mol×K	661.26	Joback Method
cpg	490.03	J/mol×K	512.80	Joback Method

dvisc	0.0077099	Pa×s	263.34	Joback Method
dvisc	0.0025488	Pa×s	304.92	Joback Method
dvisc	0.0010990	Pa×s	346.49	Joback Method
dvisc	0.0005675	Pa×s	388.07	Joback Method
dvisc	0.0003330	Pa×s	429.65	Joback Method
dvisc	0.0001486	Pa×s	512.80	Joback Method
dvisc	0.0002147	Pa×s	471.22	Joback Method
pvap	3.70e-03	kPa	277.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	4.40e-03	kPa	279.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	5.20e-03	kPa	281.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	6.20e-03	kPa	283.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	7.30e-03	kPa	285.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	9.50e-03	kPa	288.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.01	kPa	291.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.02	kPa	294.70	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	297.70	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	300.70	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	303.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559825&Units=SI

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

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