Butyl tert-octyl ether

Other names: butyl 1,1,3,3-tetramethylbutyl ether
pentane, 2-butoxy-2,4,4-trimethyl-
Inchi: InChI=1S/C12H26O/c1-7-8-9-13-12(5,6)10-11(2,3)4/h7-10H2,1-6H3
InchiKey: JVLYCQPURZKIPY-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]: 186.33

Physical Properties

Property code	Value	Unit	Source
gf	-49.16	kJ/mol	Joback Method
hf	-440.73	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	4.018		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1116.00		NIST Webbook
tb	489.92	K	Joback Method
tc	669.76	K	Joback Method
tf	252.07	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.65	J/mol×K	669.76	Joback Method
cpg	459.32	J/mol×K	519.89	Joback Method
cpg	477.30	J/mol×K	549.87	Joback Method
cpg	494.39	J/mol×K	579.84	Joback Method
cpg	510.62	J/mol×K	609.81	Joback Method
cpg	526.03	J/mol×K	639.79	Joback Method
cpg	440.40	J/mol×K	489.92	Joback Method

dvisc	0.0086566	Pa×s	252.07	Joback Method
dvisc	0.0028767	Pa×s	291.71	Joback Method
dvisc	0.0012443	Pa×s	331.35	Joback Method
dvisc	0.0006438	Pa×s	371.00	Joback Method
dvisc	0.0003783	Pa×s	410.64	Joback Method
dvisc	0.0002441	Pa×s	450.28	Joback Method
dvisc	0.0001691	Pa×s	489.92	Joback Method
pvap	0.01	kPa	278.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	281.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.02	kPa	284.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	287.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.03	kPa	290.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.04	kPa	293.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.05	kPa	296.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.07	kPa	299.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.08	kPa	302.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.10	kPa	305.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.12	kPa	308.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.15	kPa	311.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.17	kPa	314.20	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=R559672&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