

Isopropyl tert-pentyl ether

Other names:	2-methyl-2-(1-methylethoxy)butane butane, 2-methyl-2-(1-methylethoxy)- ether, isopropyl tert-pentyl
Inchi:	InChI=1S/C8H18O/c1-6-8(4,5)9-7(2)3/h7H,6H2,1-5H3
InchiKey:	WICKZWVCTKHMNG-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(C)(C)OC(C)C
Mol. weight [g/mol]:	130.23

Physical Properties

Property code	Value	Unit	Source
gf	-88.12	kJ/mol	Joback Method
hf	-354.70	kJ/mol	Joback Method
hfus	6.73	kJ/mol	Joback Method
hvap	34.13	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.600		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpola	772.00		NIST Webbook
tb	401.19	K	Joback Method
tc	579.71	K	Joback Method
tf	189.57	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.89	J/molxK	401.19	Joback Method
cpg	273.44	J/molxK	430.94	Joback Method
cpg	287.38	J/molxK	460.70	Joback Method
cpg	300.73	J/molxK	490.45	Joback Method
cpg	313.49	J/molxK	520.20	Joback Method
cpg	325.69	J/molxK	549.95	Joback Method

cpg	337.34	J/molxK	579.71	Joback Method
dvisc	0.0136359	Paxs	189.57	Joback Method
dvisc	0.0040597	Paxs	224.84	Joback Method
dvisc	0.0016788	Paxs	260.11	Joback Method
dvisc	0.0008572	Paxs	295.38	Joback Method
dvisc	0.0005052	Paxs	330.65	Joback Method
dvisc	0.0003297	Paxs	365.92	Joback Method
dvisc	0.0002319	Paxs	401.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of Branched Ethers: Experimental Study of Chemical Equilibria in the Reacting System of tert-Amyl Alkyl Ether Synthesis: McGowan Method:	https://www.doi.org/10.1021/je034172y
	https://en.wikipedia.org/wiki/Joback_method
	http://link.springer.com/article/10.1007/BF02311772

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
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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