

Pentyl tert-butyl ether

Inchi:	InChI=1S/C9H20O/c1-5-6-7-8-10-9(2,3)4/h5-8H2,1-4H3
InchiKey:	BWRSHLROMAZEEM-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCCOC(C)(C)C
Mol. weight [g/mol]:	144.25

Physical Properties

Property code	Value	Unit	Source
gf	-77.26	kJ/mol	Joback Method
hf	-370.06	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	36.74	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.992		Crippen Method
mvol	143.540	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	902.00		NIST Webbook
tb	424.51	K	Joback Method
tc	598.00	K	Joback Method
tf	215.84	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.66	J/molxK	424.51	Joback Method
cpg	370.42	J/molxK	569.09	Joback Method
cpg	357.65	J/molxK	540.17	Joback Method
cpg	344.30	J/molxK	511.26	Joback Method
cpg	330.37	J/molxK	482.34	Joback Method
cpg	315.82	J/molxK	453.43	Joback Method
cpg	382.63	J/molxK	598.00	Joback Method
dvisc	0.0002250	Paxs	424.51	Joback Method
dvisc	0.0003097	Paxs	389.73	Joback Method

dvisc	0.0004539	Paxs	354.95	Joback Method
dvisc	0.0007228	Paxs	320.17	Joback Method
dvisc	0.0012893	Paxs	285.40	Joback Method
dvisc	0.0027004	Paxs	250.62	Joback Method
dvisc	0.0071777	Paxs	215.84	Joback Method

Sources

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=R559810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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