

Isobutyl tert-pentyl ether

Inchi:

InChI=1S/C9H20O/c1-6-9(4,5)10-7-8(2)3/h8H,6-7H2,1-5H3

InchiKey:

YCTKEFKHNQHDPW-UHFFFAOYSA-N

Formula:

C9H20O

SMILES:

CCC(C)(C)OCC(C)C

Mol. weight [g/mol]:

144.25

Physical Properties

Property code	Value	Unit	Source
gf	-79.70	kJ/mol	Joback Method
hf	-375.34	kJ/mol	Joback Method
hfus	9.32	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.848		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	862.00		NIST Webbook
tb	424.07	K	Joback Method
tc	601.48	K	Joback Method
tf	200.84	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.64	J/mol×K	424.07	Joback Method
cpg	372.20	J/mol×K	571.91	Joback Method
cpg	359.13	J/mol×K	542.34	Joback Method
cpg	345.46	J/mol×K	512.77	Joback Method
cpg	331.17	J/mol×K	483.21	Joback Method
cpg	316.23	J/mol×K	453.64	Joback Method
cpg	384.67	J/mol×K	601.48	Joback Method
dvisc	0.0002159	Pa×s	424.07	Joback Method
dvisc	0.0003074	Pa×s	386.87	Joback Method

dvisc	0.0004719	Pa×s	349.66	Joback Method
dvisc	0.0008023	Pa×s	312.45	Joback Method
dvisc	0.0015744	Pa×s	275.25	Joback Method
dvisc	0.0038142	Pa×s	238.05	Joback Method
dvisc	0.0128253	Pa×s	200.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan 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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