

Heptyl tert-butyl ether

Inchi:

InChI=1S/C11H24O/c1-5-6-7-8-9-10-12-11(2,3)4/h5-10H2,1-4H3

InchiKey:

TYSCUIJRFGVUDM-UHFFFAOYSA-N

Formula:

C11H24O

SMILES:

CCCCCCCCOC(C)(C)C

Mol. weight [g/mol]:

172.31

Physical Properties

Property code	Value	Unit	Source
gf	-60.42	kJ/mol	Joback Method
hf	-411.34	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	41.19	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.772		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
tb	470.27	K	Joback Method
tc	641.42	K	Joback Method
tf	238.38	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.32	J/mol×K	470.27	Joback Method
cpg	407.21	J/mol×K	498.80	Joback Method
cpg	423.40	J/mol×K	527.32	Joback Method
cpg	438.90	J/mol×K	555.85	Joback Method
cpg	453.75	J/mol×K	584.37	Joback Method
cpg	467.95	J/mol×K	612.90	Joback Method
cpg	481.53	J/mol×K	641.42	Joback Method
dvisc	0.0065180	Pa×s	238.38	Joback Method

dvisc	0.0023977	Pa×s	277.03	Joback Method
dvisc	0.0011267	Pa×s	315.68	Joback Method
dvisc	0.0006243	Pa×s	354.32	Joback Method
dvisc	0.0003885	Pa×s	392.97	Joback Method
dvisc	0.0002632	Pa×s	431.62	Joback Method
dvisc	0.0001901	Pa×s	470.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559716&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

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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