Ether, hexyl t-butyl

Other names: Hexyl tert-butyl ether
Inchi: InChI=1S/C10H22O/c1-5-6-7-8-9-11-10(2,3)4/h5-9H2,1-4H3
InchiKey: XSBHWHZJHSUCOI-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCCOC(C)(C)C
Mol. weight [g/mol]: 158.28
CAS: 69775-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-68.84	kJ/mol	Joback Method
hf	-390.70	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	53.20	kJ/mol	NIST Webbook
log10ws	-3.21		Crippen Method
logp	3.382		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	998.00		NIST Webbook
tb	447.39	K	Joback Method
tc	619.76	K	Joback Method
tf	227.11	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.48	J/mol×K	447.39	Joback Method
cpg	360.56	J/mol×K	476.12	Joback Method
cpg	375.98	J/mol×K	504.85	Joback Method
cpg	390.75	J/mol×K	533.57	Joback Method
cpg	404.90	J/mol×K	562.30	Joback Method
cpg	418.43	J/mol×K	591.03	Joback Method
cpg	431.37	J/mol×K	619.76	Joback Method

dvisc	0.0068881	Pa×s	227.11	Joback Method
dvisc	0.0025611	Pa×s	263.82	Joback Method
dvisc	0.0012126	Pa×s	300.54	Joback Method
dvisc	0.0006756	Pa×s	337.25	Joback Method
dvisc	0.0004223	Pa×s	373.96	Joback Method
dvisc	0.0002870	Pa×s	410.68	Joback Method
dvisc	0.0002079	Pa×s	447.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69775797&Units=SI

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