

2-Hexanol, methyl ether

Inchi:	InChI=1S/C7H16O/c1-4-5-6-7(2)8-3/h7H,4-6H2,1-3H3
InchiKey:	OVLZCXHCJCDIJB-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCC(C)OC
Mol. weight [g/mol]:	116.20

Physical Properties

Property code	Value	Unit	Source
gf	-99.38	kJ/mol	Joback Method
hf	-325.31	kJ/mol	Joback Method
hfus	11.55	kJ/mol	Joback Method
hvap	33.20	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	780.10		NIST Webbook
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tb	381.54	K	Joback Method
tc	549.69	K	Joback Method
tf	175.88	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.33	J/mol×K	381.54	Joback Method
cpg	230.17	J/mol×K	409.57	Joback Method
cpg	241.65	J/mol×K	437.59	Joback Method
cpg	252.77	J/mol×K	465.62	Joback Method
cpg	263.53	J/mol×K	493.64	Joback Method
cpg	273.94	J/mol×K	521.67	Joback Method
cpg	284.00	J/mol×K	549.69	Joback Method
dvisc	0.0068890	Pa×s	175.88	Joback Method

dvisc	0.0024170	Pa×s	210.16	Joback Method
dvisc	0.0011375	Pa×s	244.43	Joback Method
dvisc	0.0006444	Pa×s	278.71	Joback Method
dvisc	0.0004135	Pa×s	312.99	Joback Method
dvisc	0.0002896	Pa×s	347.26	Joback Method
dvisc	0.0002162	Pa×s	381.54	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=U333920&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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