Hexane, 3-methoxy-3-methyl-

Inchi: InChI=1S/C8H18O/c1-5-7-8(3,6-2)9-4/h5-7H2,1-4H3
InchiKey: PCSFHUVPGSODTP-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCCC(C)(CC)OC
Mol. weight [g/mol]: 130.23
CAS: 74630-91-4

Physical Properties

Property code	Value	Unit	Source
gf	-85.68	kJ/mol	Joback Method
hf	-349.42	kJ/mol	Joback Method
hfus	10.25	kJ/mol	Joback Method
hvap	34.52	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.602		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	401.63	K	Joback Method
tc	576.09	K	Joback Method
tf	204.57	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.96	J/mol×K	401.63	Joback Method
cpg	273.09	J/mol×K	430.71	Joback Method
cpg	286.65	J/mol×K	459.78	Joback Method
cpg	299.64	J/mol×K	488.86	Joback Method
cpg	312.08	J/mol×K	517.94	Joback Method
cpg	323.99	J/mol×K	547.02	Joback Method
cpg	335.39	J/mol×K	576.09	Joback Method
dvisc	0.0073558	Pa×s	204.57	Joback Method
dvisc	0.0028037	Pa×s	237.41	Joback Method

dvisc	0.0013510	Pa×s	270.26	Joback Method
dvisc	0.0007626	Pa×s	303.10	Joback Method
dvisc	0.0004814	Pa×s	335.94	Joback Method
dvisc	0.0003298	Pa×s	368.79	Joback Method
dvisc	0.0002404	Pa×s	401.63	Joback Method

Sources

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=C74630914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume