(E)1-Methoxy-3-methyl-1-butene

Inchi: InChI=1S/C6H12O/c1-6(2)4-5-7-3/h4-6H,1-3H3/b5-4+
InchiKey: NDACTLNPNAMFLK-SNAWJCMRSA-N
Formula: C6H12O
SMILES: COC=CC(C)C
Mol. weight [g/mol]: 100.16
CAS: 31915-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-27.58	kJ/mol	Joback Method
hf	-187.45	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	30.93	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.802		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
tb	362.82	K	Joback Method
tc	540.32	K	Joback Method
tf	159.53	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.57	J/mol×K	362.82	Joback Method
cpg	177.88	J/mol×K	392.40	Joback Method
cpg	187.81	J/mol×K	421.99	Joback Method
cpg	197.37	J/mol×K	451.57	Joback Method
cpg	206.56	J/mol×K	481.15	Joback Method
cpg	215.40	J/mol×K	510.74	Joback Method
cpg	223.90	J/mol×K	540.32	Joback Method
dvisc	0.0061309	Pa×s	159.53	Joback Method
dvisc	0.0020189	Pa×s	193.41	Joback Method

dvisc	0.0009258	Pa×s	227.29	Joback Method
dvisc	0.0005198	Pa×s	261.18	Joback Method
dvisc	0.0003332	Pa×s	295.06	Joback Method
dvisc	0.0002340	Pa×s	328.94	Joback Method
dvisc	0.0001756	Pa×s	362.82	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=C31915761&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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