2-Methoxy-3-methyl-1-butene

Inchi: InChI=1S/C6H12O/c1-5(2)6(3)7-4/h5H,3H2,1-2,4H3
InchiKey: KDMASJAWKNAFBX-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=C(OC)C(C)C
Mol. weight [g/mol]: 100.16
CAS: 51776-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-28.51	kJ/mol	Joback Method
hf	-189.03	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	30.38	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.802		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	355.22	K	Joback Method
tc	530.69	K	Joback Method
tf	148.89	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.24	J/mol×K	355.22	Joback Method
cpg	178.29	J/mol×K	384.47	Joback Method
cpg	188.01	J/mol×K	413.71	Joback Method
cpg	197.41	J/mol×K	442.96	Joback Method
cpg	206.48	J/mol×K	472.20	Joback Method
cpg	215.24	J/mol×K	501.45	Joback Method
cpg	223.68	J/mol×K	530.69	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=C51776455&Units=SI

Legend

cpg:	Ideal gas heat capacity
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