1-Methoxy-3-methyl-3-butene

Other names: 4-Methoxy-2-methylbut-1-ene
Inchi: InChI=1S/C6H12O/c1-6(2)4-5-7-3/h1,4-5H2,2-3H3
InchiKey: RWOKSHXRXBYVOC-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=C(C)CCOC
Mol. weight [g/mol]: 100.16
CAS: 34752-58-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.07	kJ/mol	Joback Method
hf	-183.75	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	30.77	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.599		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	709.30		NIST Webbook
rinpol	709.30		NIST Webbook
tb	355.66	K	Joback Method
tc	526.98	K	Joback Method
tf	163.89	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.40	J/mol×K	355.66	Joback Method
cpg	178.12	J/mol×K	384.21	Joback Method
cpg	187.52	J/mol×K	412.77	Joback Method
cpg	196.63	J/mol×K	441.32	Joback Method
cpg	205.43	J/mol×K	469.87	Joback Method
cpg	213.94	J/mol×K	498.43	Joback Method

cpg	222.15	J/mol×K	526.98	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=C34752584&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume