1-Methyl-3-(hydroxy-ethyl)propadiene

Inchi: InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2,4,7H,5-6H2,1H3
InchiKey: LLCXUUIYEHIXTB-UHFFFAOYSA-N
Formula: C6H10O
SMILES: CC=C=CCCO
Mol. weight [g/mol]: 98.14

Physical Properties

Property code	Value	Unit	Source
gf	71.32	kJ/mol	Joback Method
hf	-39.40	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.100		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	819.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1194.00		NIST Webbook
tb	436.29	K	Joback Method
tc	615.22	K	Joback Method
tf	219.63	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.85	J/mol×K	436.29	Joback Method
cpg	188.05	J/mol×K	466.11	Joback Method
cpg	195.93	J/mol×K	495.93	Joback Method
cpg	203.48	J/mol×K	525.76	Joback Method

cpg	210.73	J/mol×K	555.58	Joback Method
cpg	217.67	J/mol×K	585.40	Joback Method
cpg	224.32	J/mol×K	615.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292101&Units=SI
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

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