3-Methylpenta-1,4-diene-3-ol

Inchi: InChI=1S/C6H10O/c1-4-6(3,7)5-2/h4-5,7H,1-2H2,3H3
InchiKey: LNSCVZRMAHCQIH-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C=CC(C)(O)C=C
Mol. weight [g/mol]: 98.14
CAS: 918-86-5

Physical Properties

Property code	Value	Unit	Source
gf	41.34	kJ/mol	Joback Method
hf	-77.29	kJ/mol	Joback Method
hfus	5.41	kJ/mol	Joback Method
hvap	42.99	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.109		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	824.00		NIST Webbook
rinpol	824.00		NIST Webbook
tb	418.99	K	Joback Method
tc	597.06	K	Joback Method
tf	217.10	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.23	J/mol×K	418.99	Joback Method
cpg	188.60	J/mol×K	448.67	Joback Method
cpg	197.42	J/mol×K	478.35	Joback Method
cpg	205.71	J/mol×K	508.03	Joback Method
cpg	213.51	J/mol×K	537.71	Joback Method
cpg	220.84	J/mol×K	567.39	Joback Method
cpg	227.73	J/mol×K	597.06	Joback Method

dvisc	0.1123776	Pa×s	217.10	Joback Method
dvisc	0.0211100	Pa×s	250.75	Joback Method
dvisc	0.0058903	Pa×s	284.40	Joback Method
dvisc	0.0021532	Pa×s	318.04	Joback Method
dvisc	0.0009542	Pa×s	351.69	Joback Method
dvisc	0.0004875	Pa×s	385.34	Joback Method
dvisc	0.0002774	Pa×s	418.99	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=C918865&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume