4-Methylcyclohexanol acetate

Other names: 4-Methylcyclohexyl acetate
Inchi: InChI=1S/C9H16O2/c1-7-3-5-9(6-4-7)11-8(2)10/h7,9H,3-6H2,1-2H3/t7-,9-
InchiKey: VJBFCCCTSQEGMH-XWEPSHTISA-N
Formula: C9H16O2
SMILES: CC(=O)OC1CCC(C)CC1
Mol. weight [g/mol]: 156.22
CAS: 22597-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-192.28	kJ/mol	Joback Method
hf	-439.91	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	54.10	kJ/mol	NIST Webbook
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	496.49	K	Joback Method
tc	704.73	K	Joback Method
tf	266.49	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.98	J/mol×K	496.49	Joback Method
cpg	326.41	J/mol×K	531.20	Joback Method
cpg	343.02	J/mol×K	565.90	Joback Method
cpg	358.81	J/mol×K	600.61	Joback Method
cpg	373.79	J/mol×K	635.31	Joback Method
cpg	387.96	J/mol×K	670.02	Joback Method
cpg	401.32	J/mol×K	704.73	Joback Method
dvisc	0.0031798	Pa×s	266.49	Joback Method

dvisc	0.0016403	Pa×s	304.82	Joback Method
dvisc	0.0009810	Pa×s	343.16	Joback Method
dvisc	0.0006505	Pa×s	381.49	Joback Method
dvisc	0.0004650	Pa×s	419.82	Joback Method
dvisc	0.0003516	Pa×s	458.16	Joback Method
dvisc	0.0002776	Pa×s	496.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22597235&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
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