CYCLOHEXANOL, 1-METHYL-, ACETATE

Other names: 1-Methylcyclohexyl acetate
Inchi: InChI=1S/C9H16O2/c1-8(10)11-9(2)6-4-3-5-7-9/h3-7H2,1-2H3
InchiKey: VVDZWMOQABVVHC-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC(=O)OC1(C)CCCCC1
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
hfus	7.39	kJ/mol	Joback Method
hvap	52.40	kJ/mol	NIST Webbook
ie	9.67	eV	Cheméo Relay (1.0)
logp	2.272		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
tb	444.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.50	J/mol×K	501.40	Joback Method
cpg	325.53	J/mol×K	537.63	Joback Method
cpg	341.50	J/mol×K	573.86	Joback Method
cpg	356.52	J/mol×K	610.09	Joback Method
cpg	370.67	J/mol×K	646.32	Joback Method
cpg	384.06	J/mol×K	682.55	Joback Method
cpg	396.78	J/mol×K	718.78	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16737307&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature