3-Cyclohexen-1-ol, acetate

Other names:	3-Cyclohexen-1-yl acetate
	3-Cyclohexenyl acetate
	4-Acetoxycyclohexene
Inchi:	InChI=1S/C8H12O2/c1-7(9)10-8-5-3-2-4-6-8/h2-3,8H,4-6H2,1H3
InchiKey:	IIOLXIVFODJEDX-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC(=O)OC1CC=CCC1
Mol. weight [g/mol]:	140.18
CAS:	10437-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-163.03	kJ/mol	Joback Method
hf	-341.15	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	43.28	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1010.00		NIST Webbook
rinpol	1010.00		NIST Webbook
tb	477.44	K	Joback Method
tc	691.16	K	Joback Method
tf	260.22	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.26	J/mol×K	477.44	Joback Method
cpg	262.12	J/mol×K	513.06	Joback Method
cpg	276.22	J/mol×K	548.68	Joback Method
cpg	289.57	J/mol×K	584.30	Joback Method

cpg	302.19	J/mol×K	619.92	Joback Method
cpg	314.08	J/mol×K	655.54	Joback Method
cpg	325.25	J/mol×K	691.16	Joback Method
dvisc	0.0035229	Pa×s	260.22	Joback Method
dvisc	0.0017750	Pa×s	296.42	Joback Method
dvisc	0.0010382	Pa×s	332.63	Joback Method
dvisc	0.0006747	Pa×s	368.83	Joback Method
dvisc	0.0004736	Pa×s	405.03	Joback Method
dvisc	0.0003523	Pa×s	441.24	Joback Method
dvisc	0.0002741	Pa×s	477.44	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=C10437782&Units=SI

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

Latest version available from: