3-Cyclohex-1-enyl-prop-2-enal

Other names: 2-Propenal, 3-(1-cyclohexenyl)
Inchi: InChI=1S/C9H12O/c10-8-4-7-9-5-2-1-3-6-9/h4-5,7-8H,1-3,6H2/b7-4+
InchiKey: JGUXSPMZBDGHFV-QPJJXVBHSA-N
Formula: C9H12O
SMILES: O=CC=CC1=CCCCC1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
gf	58.09	kJ/mol	Joback Method
hf	-76.48	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	44.00	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.242		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1001.00		NIST Webbook
rinpol	1001.00		NIST Webbook
tb	486.50	K	Joback Method
tc	705.22	K	Joback Method
tf	253.01	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.09	J/mol×K	486.50	Joback Method
cpg	264.77	J/mol×K	522.95	Joback Method
cpg	278.51	J/mol×K	559.41	Joback Method
cpg	291.36	J/mol×K	595.86	Joback Method
cpg	303.37	J/mol×K	632.31	Joback Method
cpg	314.59	J/mol×K	668.77	Joback Method
cpg	325.06	J/mol×K	705.22	Joback Method

dvisc	0.0048247	Pa×s	253.01	Joback Method
dvisc	0.0021302	Pa×s	291.93	Joback Method
dvisc	0.0011400	Pa×s	330.84	Joback Method
dvisc	0.0006958	Pa×s	369.75	Joback Method
dvisc	0.0004666	Pa×s	408.67	Joback Method
dvisc	0.0003354	Pa×s	447.58	Joback Method
dvisc	0.0002542	Pa×s	486.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U193702&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume