2H-Pyran-2-carboxaldehyde, 3,4-dihydro-

Other names:	Acrolein dimer
	2-Propenal dimer
	5-Hexenal, 2,6-epoxy-
	Pyran aldehyde
	2-Formyl-3,4-dihydro-2H-pyran
	3,4-Dihydro-2H-pyran-2-carboxaldehyde
	2,3-Dihydro-1,4-pyran-2-karboxaldehyd
	3,4-Dihydro-2-carboxaldehyde-2H-pyran
	3,4-Dihydro-2-formyl-2H-pyran
	NSC 95413
	Acroleine dimer
	3,4-dihydro-2H-pyran-2-carbaldehyde
Inchi:	InChI=1S/C6H8O2/c7-5-6-3-1-2-4-8-6/h2,4-6H,1,3H2
InchiKey:	NPWYTMFWRRIFLK-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	O=CC1CCC=CO1
Mol. weight [g/mol]:	112.13
CAS:	100-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-131.59	kJ/mol	Joback Method
hf	-272.65	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	40.90	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
rinpol	853.00		NIST Webbook
tb	431.00	K	Joback Method
tc	645.54	K	Joback Method
tf	234.09	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.89	J/mol×K	431.00	Joback Method
cpg	225.35	J/mol×K	609.79	Joback Method
cpg	215.92	J/mol×K	574.03	Joback Method
cpg	205.88	J/mol×K	538.27	Joback Method
cpg	195.21	J/mol×K	502.51	Joback Method
cpg	183.88	J/mol×K	466.76	Joback Method
cpg	234.17	J/mol×K	645.54	Joback Method
dvisc	0.0003989	Pa×s	431.00	Joback Method
dvisc	0.0005138	Pa×s	398.18	Joback Method
dvisc	0.0006925	Pa×s	365.36	Joback Method
dvisc	0.0009901	Pa×s	332.54	Joback Method
dvisc	0.0015308	Pa×s	299.73	Joback Method
dvisc	0.0026345	Pa×s	266.91	Joback Method
dvisc	0.0052794	Pa×s	234.09	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100732&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

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