3-Cyclohexene-1-carboxaldehyde

Other names:	Cyclohexene-4-carboxaldehyde
	1-Formyl-3-cyclohexene
	1,2,3,6-Tetrahydrobenzaldehyde
	1,2,5,6-Tetrahydrobenzaldehyde
	3-Cyclohexen-1-aldehyde
	4-Formylcyclohexene
	1,2,3,6-Tetrahydrobenzaldehyde(1,2,5,6)
	1-Cyclohexene-4-carboxaldehyde
	4-Cyclohexene-1-carboxaldehyde
	UN 2498
	NSC 16241
	cyclohex-3-ene-1-carbaldehyde
Inchi:	InChI=1S/C7H10O/c8-6-7-4-2-1-3-5-7/h1-2,6-7H,3-5H2
InchiKey:	DCFDVJPDXYGCOK-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	O=CC1CC=CCC1
Mol. weight [g/mol]:	110.15
CAS:	100-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-37.05	kJ/mol	Joback Method
hf	-161.29	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	38.62	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
ripol	1490.00		NIST Webbook
tb	437.00 ± 3.00	K	NIST Webbook
tb	438.15	K	NIST Webbook
tb	437.20	K	NIST Webbook
tc	639.30	K	Joback Method
tf	177.10 ± 1.00	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.25	J/mol×K	426.93	Joback Method
cpg	196.95	J/mol×K	462.32	Joback Method
cpg	209.90	J/mol×K	497.72	Joback Method
cpg	222.11	J/mol×K	533.11	Joback Method
cpg	233.61	J/mol×K	568.51	Joback Method
cpg	244.42	J/mol×K	603.90	Joback Method
cpg	254.56	J/mol×K	639.30	Joback Method
dvisc	0.0049031	Pa×s	218.79	Joback Method
dvisc	0.0023281	Pa×s	253.48	Joback Method
dvisc	0.0013226	Pa×s	288.17	Joback Method
dvisc	0.0008484	Pa×s	322.86	Joback Method
dvisc	0.0005932	Pa×s	357.55	Joback Method
dvisc	0.0004419	Pa×s	392.24	Joback Method
dvisc	0.0003453	Pa×s	426.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.20	K	1.70	NIST Webbook

Sources

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=C100505&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume