Cyclohexanecarboxaldehyde

Other names:	Cyclohexanal
	Cyclohexanaldehyde
	Cyclohexanealdehyde
	Cyclohexylcarboxaldehyde
	Cyclohexylformaldehyde
	Formylcyclohexane
	1-Formylcyclohexane
	Cyclohexane-1-carboxaldehyde
	Cyclohexanecarbaldehyde
	Cyclohexylmethanal
	Hexahydrobenzaldehyde
	1-Cyclohexanecarboxaldehyde
	NSC 68509
Inchi:	InChI=1S/C7H12O/c8-6-7-4-2-1-3-5-7/h6-7H,1-5H2
InchiKey:	KVFDZFBHBWTVID-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	O=CC1CCCCC1
Mol. weight [g/mol]:	112.17
CAS:	2043-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-67.01	kJ/mol	Joback Method
hf	-219.07	kJ/mol	Joback Method
hfus	8.01	kJ/mol	Joback Method
hvap	38.33	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	965.00		NIST Webbook
ripol	1527.00		NIST Webbook
tb	435.20	K	NIST Webbook
tb	432.50	K	NIST Webbook

tc	637.91	K	Joback Method
tf	218.03	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.10	J/mol×K	427.77	Joback Method
cpg	212.12	J/mol×K	462.79	Joback Method
cpg	226.36	J/mol×K	497.82	Joback Method
cpg	239.83	J/mol×K	532.84	Joback Method
cpg	252.56	J/mol×K	567.87	Joback Method
cpg	264.56	J/mol×K	602.89	Joback Method
cpg	275.85	J/mol×K	637.91	Joback Method
dvisc	0.0065154	Pa×s	218.03	Joback Method
dvisc	0.0028831	Pa×s	252.99	Joback Method
dvisc	0.0015551	Pa×s	287.94	Joback Method
dvisc	0.0009587	Pa×s	322.90	Joback Method
dvisc	0.0006497	Pa×s	357.86	Joback Method
dvisc	0.0004718	Pa×s	392.81	Joback Method
dvisc	0.0003610	Pa×s	427.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.50 ± 0.50	K	2.70	NIST Webbook

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=C2043610&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
ie:	Ionization energy
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
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