

1-Cyclohexene-1-carboxylic acid

Other names:	1-Cyclohexenecarboxylic acid
Inchi:	InChI=1S/C7H10O2/c8-7(9)6-4-2-1-3-5-6/h4H,1-3,5H2,(H,8,9)
InchiKey:	NMEZJSDUZQOPFE-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	O=C(O)C1=CCCCC1
Mol. weight [g/mol]:	126.15
CAS:	636-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-205.19	kJ/mol	Joback Method
hf	-331.65	kJ/mol	Joback Method
hfus	11.17	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.571		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	533.97	K	Joback Method
tc	739.57	K	Joback Method
tf	304.30	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.13	J/mol×K	533.97	Joback Method
cpg	241.13	J/mol×K	568.24	Joback Method
cpg	251.49	J/mol×K	602.50	Joback Method
cpg	261.24	J/mol×K	636.77	Joback Method
cpg	270.39	J/mol×K	671.03	Joback Method
cpg	278.97	J/mol×K	705.30	Joback Method
cpg	287.00	J/mol×K	739.57	Joback Method
dvisc	0.0126756	Pa×s	304.30	Joback Method

dvisc	0.0039719	Pa×s	342.58	Joback Method
dvisc	0.0015716	Pa×s	380.86	Joback Method
dvisc	0.0007366	Pa×s	419.13	Joback Method
dvisc	0.0003919	Pa×s	457.41	Joback Method
dvisc	0.0002299	Pa×s	495.69	Joback Method
dvisc	0.0001455	Pa×s	533.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.00 ± 1.00	K	1.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C636828&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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