3-Cyclohexene-1-carboxylic acid

Other names:	«delta»3-Cyclohexenecarboxylic acid
	«delta»3-Cyclohexenylcarboxylic acid
	1-Cyclohexene-4-carboxylic acid
	3-Cyclohexenecarboxylic acid
	1,2,3,6-Tetrahydrobenzoic acid
	Kyselina 1,2,5,6-tetrahydrobenzoova
	NSC 44712
	NSC 44883
	cyclohex-3-ene-1-carboxylic acid
Inchi:	InChI=1S/C7H10O2/c8-7(9)6-4-2-1-3-5-6/h1-2,6H,3-5H2,(H,8,9)
InchiKey:	VUSWCWPCANWBFG-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	O=C(O)C1CC=CCC1
Mol. weight [g/mol]:	126.15
CAS:	4771-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-203.27	kJ/mol	Joback Method
hf	-340.52	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
ripol	1360.00		NIST Webbook
tb	524.32	K	Joback Method
tc	728.64	K	Joback Method
tf	287.54	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.18	J/mol×K	524.32	Joback Method
cpg	243.89	J/mol×K	558.37	Joback Method
cpg	254.93	J/mol×K	592.43	Joback Method
cpg	265.31	J/mol×K	626.48	Joback Method
cpg	275.06	J/mol×K	660.53	Joback Method
cpg	284.19	J/mol×K	694.59	Joback Method
cpg	292.72	J/mol×K	728.64	Joback Method
dvisc	0.0181175	Pa×s	287.54	Joback Method
dvisc	0.0052223	Pa×s	327.00	Joback Method
dvisc	0.0019678	Pa×s	366.47	Joback Method
dvisc	0.0008964	Pa×s	405.93	Joback Method
dvisc	0.0004694	Pa×s	445.39	Joback Method
dvisc	0.0002731	Pa×s	484.86	Joback Method
dvisc	0.0001724	Pa×s	524.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.50 ± 1.50	K	2.40	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=C4771806&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
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