

3-Cyclohexenecarbonyl chloride

Inchi:	InChI=1S/C7H9ClO/c8-7(9)6-4-2-1-3-5-6/h1-2,6H,3-5H2
InchiKey:	CXWMHIRIXVNVQN-UHFFFAOYSA-N
Formula:	C7H9ClO
SMILES:	O=C(Cl)C1CC=CCC1
Mol. weight [g/mol]:	144.60
CAS:	932-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-78.38	kJ/mol	Joback Method
hf	-204.03	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.108		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	469.57	K	Joback Method
tc	694.75	K	Joback Method
tf	256.64	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.82	J/mol×K	469.57	Joback Method
cpg	267.95	J/mol×K	657.22	Joback Method
cpg	257.69	J/mol×K	619.69	Joback Method
cpg	246.67	J/mol×K	582.16	Joback Method
cpg	234.87	J/mol×K	544.63	Joback Method
cpg	222.27	J/mol×K	507.10	Joback Method
cpg	277.49	J/mol×K	694.75	Joback Method
dvisc	0.0003618	Paxs	469.57	Joback Method
dvisc	0.0004629	Paxs	434.08	Joback Method

dvisc	0.0006189	Paxs	398.59	Joback Method
dvisc	0.0008757	Paxs	363.11	Joback Method
dvisc	0.0013359	Paxs	327.62	Joback Method
dvisc	0.0022580	Paxs	292.13	Joback Method
dvisc	0.0044130	Paxs	256.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.50 ± 1.50	K	2.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932672&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
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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