3-Chloro-2-norbornanone

Other names: Bicyclo[2.2.1]heptan-2-one, 3-chloro-, endo-
3-chloronorbornan-2-one
Inchi: InChI=1S/C7H9ClO/c8-6-4-1-2-5(3-4)7(6)9/h4-6H,1-3H2
InchiKey: PQRKEKMZLKKQOP-UHFFFAOYSA-N
Formula: C7H9ClO
SMILES: O=C1C2CCC(C2)C1Cl
Mol. weight [g/mol]: 144.60
CAS: 30860-22-1

Physical Properties

Property code	Value	Unit	Source
gf	-24.77	kJ/mol	Joback Method
hf	-222.15	kJ/mol	Joback Method
hfus	12.83	kJ/mol	Joback Method
hvap	39.50	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.593		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	477.89	K	Joback Method
tc	708.32	K	Joback Method
tf	294.91	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.65	J/mol×K	477.89	Joback Method
cpg	234.41	J/mol×K	516.30	Joback Method
cpg	248.27	J/mol×K	554.70	Joback Method
cpg	261.27	J/mol×K	593.11	Joback Method
cpg	273.45	J/mol×K	631.51	Joback Method
cpg	284.85	J/mol×K	669.92	Joback Method
cpg	295.50	J/mol×K	708.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	1.30	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=C30860221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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