5-Chloro-1-indanone

Other names: 1H-Inden-1-one, 5-chloro-2,3-dihydro-
1-Indanone, 5-chloro-
5-Chloro-2,3-dihydro-1H-inden-1-one
5-Chloro-indan-1-one
Inchi: InChI=1S/C9H7ClO/c10-7-2-3-8-6(5-7)1-4-9(8)11/h2-3,5H,1,4H2
InchiKey: MEDSHTHCZIOVPU-UHFFFAOYSA-N
Formula: C9H7ClO
SMILES: O=C1CCc2cc(Cl)ccc21
Mol. weight [g/mol]: 166.60
CAS: 42348-86-7

Physical Properties

Property code	Value	Unit	Source
gf	51.99	kJ/mol	Joback Method
hf	-75.80	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.469		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	558.62	K	Joback Method
tc	809.60	K	Joback Method
tf	362.97	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.71	J/mol×K	558.62	Joback Method
cpg	259.92	J/mol×K	600.45	Joback Method
cpg	271.27	J/mol×K	642.28	Joback Method
cpg	281.81	J/mol×K	684.11	Joback Method
cpg	291.58	J/mol×K	725.94	Joback Method

cpg	300.62	J/mol×K	767.77	Joback Method
cpg	308.98	J/mol×K	809.60	Joback Method

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=C42348867&Units=SI

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