3-Chloro-4-phenyl-3-butene-2-one

Inchi: InChI=1S/C10H9ClO/c1-8(12)10(11)7-9-5-3-2-4-6-9/h2-7H,1H3/b10-7-
InchiKey: XHVFFQBYESFJLP-YFHOEESVSA-N
Formula: C10H9ClO
SMILES: CC(=O)C(Cl)=Cc1ccccc1
Mol. weight [g/mol]: 180.63
CAS: 53973-14-1

Physical Properties

Property code	Value	Unit	Source
gf	76.55	kJ/mol	Joback Method
hf	-34.09	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.855		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	550.22	K	Joback Method
tc	784.68	K	Joback Method
tf	289.69	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.83	J/mol×K	550.22	Joback Method
cpg	296.46	J/mol×K	589.30	Joback Method
cpg	308.11	J/mol×K	628.37	Joback Method
cpg	318.86	J/mol×K	667.45	Joback Method
cpg	328.78	J/mol×K	706.52	Joback Method
cpg	337.93	J/mol×K	745.60	Joback Method
cpg	346.37	J/mol×K	784.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53973141&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
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