o-Chlorophenyl cyclopentyl ketone

Other names: 2-Chlorophenyl cyclopentyl ketone
Methanone, (2-chlorophenyl)cyclopentyl-
Inchi: InChI=1S/C12H13ClO/c13-11-8-4-3-7-10(11)12(14)9-5-1-2-6-9/h3-4,7-9H,1-2,5-6H2
InchiKey: QIJMMRNZBJHXRI-UHFFFAOYSA-N
Formula: C12H13ClO
SMILES: O=C(c1ccccc1Cl)C1CCCC1
Mol. weight [g/mol]: 208.68
CAS: 6740-85-8

Physical Properties

Property code	Value	Unit	Source
gf	48.64	kJ/mol	Joback Method
hf	-133.79	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.713		Crippen Method
mcvol	159.130	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	612.20	K	Joback Method
tc	857.24	K	Joback Method
tf	354.69	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.99	J/mol×K	612.20	Joback Method
cpg	455.18	J/mol×K	816.40	Joback Method
cpg	443.23	J/mol×K	775.56	Joback Method
cpg	430.21	J/mol×K	734.72	Joback Method
cpg	416.04	J/mol×K	693.88	Joback Method
cpg	400.66	J/mol×K	653.04	Joback Method
cpg	466.11	J/mol×K	857.24	Joback Method

dvisc	0.0003066	Pa×s	612.20	Joback Method
dvisc	0.0003803	Pa×s	569.28	Joback Method
dvisc	0.0004887	Pa×s	526.36	Joback Method
dvisc	0.0006566	Pa×s	483.45	Joback Method
dvisc	0.0009345	Pa×s	440.53	Joback Method
dvisc	0.0014351	Pa×s	397.61	Joback Method
dvisc	0.0024451	Pa×s	354.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.50 ± 0.50	K	0.04	NIST Webbook

Sources

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=C6740858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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