3-Pentanone, 2,2-dichloro

Inchi: InChI=1S/C5H8Cl2O/c1-3-4(8)5(2,6)7/h3H2,1-2H3
InchiKey: BMDBRMSPWDBXGN-UHFFFAOYSA-N
Formula: C5H8Cl2O
SMILES: CCC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]: 155.02

Physical Properties

Property code	Value	Unit	Source
gf	-158.72	kJ/mol	Joback Method
hf	-299.34	kJ/mol	Joback Method
hfus	11.29	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.159		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	439.30	K	Joback Method
tc	645.91	K	Joback Method
tf	258.30	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.93	J/mol×K	439.30	Joback Method
cpg	201.14	J/mol×K	473.73	Joback Method
cpg	209.74	J/mol×K	508.17	Joback Method
cpg	217.75	J/mol×K	542.60	Joback Method
cpg	225.21	J/mol×K	577.04	Joback Method
cpg	232.16	J/mol×K	611.47	Joback Method
cpg	238.61	J/mol×K	645.91	Joback Method
dvisc	0.0053482	Pa×s	258.30	Joback Method

dvisc	0.0027862	Pa×s	288.47	Joback Method
dvisc	0.0016423	Pa×s	318.63	Joback Method
dvisc	0.0010607	Pa×s	348.80	Joback Method
dvisc	0.0007344	Pa×s	378.97	Joback Method
dvisc	0.0005369	Pa×s	409.13	Joback Method
dvisc	0.0004097	Pa×s	439.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630330&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume