3-Pentanone, 2,4-dichloro-2-methyl

Inchi: InChI=1S/C6H10Cl2O/c1-4(7)5(9)6(2,3)8/h4H,1-3H3
InchiKey: OLIGKRNGLJKEAV-UHFFFAOYSA-N
Formula: C6H10Cl2O
SMILES: CC(Cl)C(=O)C(C)(C)Cl
Mol. weight [g/mol]: 169.05

Physical Properties

Property code	Value	Unit	Source
gf	-152.74	kJ/mol	Joback Method
hf	-325.26	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.200		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	942.00		NIST Webbook
rinpol	942.00		NIST Webbook
tb	461.74	K	Joback Method
tc	670.58	K	Joback Method
tf	254.57	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.86	J/mol×K	461.74	Joback Method
cpg	241.62	J/mol×K	496.55	Joback Method
cpg	251.67	J/mol×K	531.35	Joback Method
cpg	261.06	J/mol×K	566.16	Joback Method
cpg	269.82	J/mol×K	600.97	Joback Method
cpg	277.98	J/mol×K	635.77	Joback Method
cpg	285.58	J/mol×K	670.58	Joback Method
dvisc	0.0076920	Pa×s	254.57	Joback Method

dvisc	0.0033961	Pa×s	289.10	Joback Method
dvisc	0.0017852	Pa×s	323.63	Joback Method
dvisc	0.0010623	Pa×s	358.15	Joback Method
dvisc	0.0006925	Pa×s	392.68	Joback Method
dvisc	0.0004838	Pa×s	427.21	Joback Method
dvisc	0.0003566	Pa×s	461.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630350&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