3-Pentanone, 2,2,4-trichloro

Inchi: InChI=1S/C5H7Cl3O/c1-3(6)4(9)5(2,7)8/h3H,1-2H3
InchiKey: RJGCDEWEOGDQBQ-UHFFFAOYSA-N
Formula: C5H7Cl3O
SMILES: CC(Cl)C(=O)C(C)(Cl)Cl
Mol. weight [g/mol]: 189.47

Physical Properties

Property code	Value	Unit	Source
gf	-173.09	kJ/mol	Joback Method
hf	-320.36	kJ/mol	Joback Method
hfus	11.96	kJ/mol	Joback Method
hvap	44.94	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.377		Crippen Method
mcvol	119.600	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	476.29	K	Joback Method
tc	694.32	K	Joback Method
tf	273.22	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.62	J/mol×K	476.29	Joback Method
cpg	252.54	J/mol×K	657.98	Joback Method
cpg	246.14	J/mol×K	621.64	Joback Method
cpg	239.19	J/mol×K	585.31	Joback Method
cpg	231.64	J/mol×K	548.97	Joback Method
cpg	223.47	J/mol×K	512.63	Joback Method
cpg	258.43	J/mol×K	694.32	Joback Method
dvisc	0.0003809	Pa×s	476.29	Joback Method

dvisc	0.0005101	Pa×s	442.45	Joback Method
dvisc	0.0007172	Pa×s	408.60	Joback Method
dvisc	0.0010723	Pa×s	374.75	Joback Method
dvisc	0.0017365	Pa×s	340.91	Joback Method
dvisc	0.0031276	Pa×s	307.07	Joback Method
dvisc	0.0065167	Pa×s	273.22	Joback Method

Sources

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=R630325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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