1,1,1,3-tetrachloropropanone

Other names: 1,1,1,3-Tetrachloro-2-propanone
1,1,1,3-Tetrachloroacetone
1,1,1,3-Tetrachloropropanone
Inchi: InChI=1S/C3H2Cl4O/c4-1-2(8)3(5,6)7/h1H2
InchiKey: MSZQBKOLHPDFFD-UHFFFAOYSA-N
Formula: C3H2Cl4O
SMILES: O=C(CCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 195.86

Physical Properties

Property code	Value	Unit	Source
hf	-258.01	kJ/mol	Cheméo Relay (1.0)
hfus	14.50	kJ/mol	Joback Method
ie	10.32	eV	Cheméo Relay (1.0)
log10ws	-2.09		Cheméo Relay (1.0)
logp	2.164		Crippen Method
mcvol	103.660	ml/mol	McGowan Method
rinpol	1009.00		NIST Webbook
tb	449.93	K	Cheméo Relay (1.0)
tf	289.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.04	J/mol×K	468.40	Joback Method
cpg	164.20	J/mol×K	506.03	Joback Method
cpg	168.83	J/mol×K	543.66	Joback Method
cpg	172.97	J/mol×K	581.29	Joback Method
cpg	176.66	J/mol×K	618.92	Joback Method
cpg	179.94	J/mol×K	656.55	Joback Method
cpg	182.86	J/mol×K	694.18	Joback Method
dvisc	0.0042880	Pa×s	295.60	Joback Method
dvisc	0.0025238	Pa×s	324.40	Joback Method
dvisc	0.0016195	Pa×s	353.20	Joback Method

dvisc	0.0011111	Pa×s	382.00	Joback Method
dvisc	0.0008037	Pa×s	410.80	Joback Method
dvisc	0.0006065	Pa×s	439.60	Joback Method
dvisc	0.0004739	Pa×s	468.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16995350&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point