

2-Butanone, 1,3,3,4-tetrachloro

Inchi: InChI=1S/C4H4Cl4O/c5-1-3(9)4(7,8)2-6/h1-2H2
InchiKey: FOKWKGKSYBDIIRQ-UHFFFAOYSA-N
Formula: C4H4Cl4O
SMILES: O=C(CCl)C(Cl)(Cl)CCl
Mol. weight [g/mol]: 209.89

Physical Properties

Property code	Value	Unit	Source
gf	-191.00	kJ/mol	Joback Method
hf	-310.18	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	47.49	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.207		Crippen Method
mcvol	117.750	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
tb	491.28	K	Joback Method
tc	713.40	K	Joback Method
tf	306.87	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.28	J/molxK	491.28	Joback Method
cpg	202.85	J/molxK	528.30	Joback Method
cpg	208.83	J/molxK	565.32	Joback Method
cpg	214.27	J/molxK	602.34	Joback Method
cpg	219.20	J/molxK	639.36	Joback Method

cpg	223.66	J/molxK	676.38	Joback Method
cpg	227.71	J/molxK	713.40	Joback Method
dvisc	0.0041106	Paxs	306.87	Joback Method
dvisc	0.0023680	Paxs	337.61	Joback Method
dvisc	0.0014956	Paxs	368.34	Joback Method
dvisc	0.0010139	Paxs	399.07	Joback Method
dvisc	0.0007267	Paxs	429.81	Joback Method
dvisc	0.0005445	Paxs	460.54	Joback Method
dvisc	0.0004230	Paxs	491.28	Joback Method

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=R629484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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