

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

Inchi:	InChI=1S/C4H4Cl4O/c1-2(5)3(9)4(6,7)8/h2H,1H3
InchiKey:	XUXXNYSMGGGDNV-UHFFFAOYSA-N
Formula:	C4H4Cl4O
SMILES:	CC(Cl)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	209.89

Physical Properties

Property code	Value	Unit	Source
gf	-193.44	kJ/mol	Joback Method
hf	-315.46	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.553		Crippen Method
mcvol	117.750	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1024.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1024.00		NIST Webbook
tb	490.84	K	Joback Method
tc	718.27	K	Joback Method
tf	291.87	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.59	J/mol×K	490.84	Joback Method
cpg	203.41	J/mol×K	528.75	Joback Method
cpg	209.59	J/mol×K	566.65	Joback Method
cpg	215.19	J/mol×K	604.56	Joback Method
cpg	220.26	J/mol×K	642.46	Joback Method

cpg	224.83	J/mol×K	680.37	Joback Method
cpg	228.95	J/mol×K	718.27	Joback Method
dvisc	0.0055872	Paxs	291.87	Joback Method
dvisc	0.0028789	Paxs	325.03	Joback Method
dvisc	0.0016772	Paxs	358.19	Joback Method
dvisc	0.0010707	Paxs	391.36	Joback Method
dvisc	0.0007332	Paxs	424.52	Joback Method
dvisc	0.0005304	Paxs	457.68	Joback Method
dvisc	0.0004009	Paxs	490.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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