

2-CYCLOBUTEN-1-ONE, 2,3,4,4-TETRACHLORO-

Other names:	2-Cyclobuten-1-one, 2,3,4,4-tetrachloro- Perchloro-2-cyclobuten-1-one Perchloro-2-cyclobutene-1-one Perchlorocyclobut-2-enone Tetrachlorocyclobutenone tetrachlorocyclobut-2-enone
Inchi:	InChI=1S/C4Cl4O/c5-1-2(6)4(7,8)3(1)9
InchiKey:	NWDONRNKYCKRNT-UHFFFAOYSA-N
Formula:	C4Cl4O
SMILES:	O=C1C(Cl)=C(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	205.86

Physical Properties

Property code	Value	Unit	Source
hf	-94.32	kJ/mol	Cheméo Relay (1.0)
hfus	12.60	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.23		Cheméo Relay (1.0)
logp	2.432		Crippen Method
mcvol	102.590	ml/mol	McGowan Method
tb	461.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.47	J/mol×K	528.83	Joback Method
cpg	164.01	J/mol×K	571.67	Joback Method
cpg	168.16	J/mol×K	614.50	Joback Method
cpg	172.03	J/mol×K	657.34	Joback Method
cpg	175.78	J/mol×K	700.18	Joback Method
cpg	179.52	J/mol×K	743.02	Joback Method
cpg	183.39	J/mol×K	785.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3200962&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature

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