

2-Pentanone, 1,1-dichloro

Inchi:	InChI=1S/C5H8Cl2O/c1-2-3-4(8)5(6)7/h5H,2-3H2,1H3
InchiKey:	QDGHMJDTBJTMRN-UHFFFAOYSA-N
Formula:	C5H8Cl2O
SMILES:	CCCC(=O)C(Cl)Cl
Mol. weight [g/mol]:	155.02

Physical Properties

Property code	Value	Unit	Source
gf	-164.00	kJ/mol	Joback Method
hf	-295.87	kJ/mol	Joback Method
hfus	15.18	kJ/mol	Joback Method
hvap	41.85	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.159		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	442.09	K	Joback Method
tc	640.12	K	Joback Method
tf	240.88	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.18	J/molxK	442.09	Joback Method
cpg	197.60	J/molxK	475.09	Joback Method
cpg	205.61	J/molxK	508.10	Joback Method
cpg	213.21	J/molxK	541.10	Joback Method
cpg	220.41	J/molxK	574.11	Joback Method
cpg	227.23	J/molxK	607.11	Joback Method
cpg	233.68	J/molxK	640.12	Joback Method
dvisc	0.0053985	Paxs	240.88	Joback Method

dvisc	0.0026428	Paxs	274.42	Joback Method
dvisc	0.0015116	Paxs	307.95	Joback Method
dvisc	0.0009648	Paxs	341.49	Joback Method
dvisc	0.0006673	Paxs	375.02	Joback Method
dvisc	0.0004903	Paxs	408.56	Joback Method
dvisc	0.0003776	Paxs	442.09	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=R629939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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