

3-Pentanone, 2,4-dichloro (RR, SS)

Inchi:	InChI=1S/C5H8Cl2O/c1-3(6)5(8)4(2)7/h3-4H,1-2H3
InchiKey:	XNTVDJIRXYIWQH-UHFFFAOYSA-N
Formula:	C5H8Cl2O
SMILES:	CC(Cl)C(=O)C(C)Cl
Mol. weight [g/mol]:	155.02

Physical Properties

Property code	Value	Unit	Source
gf	-166.44	kJ/mol	Joback Method
hf	-301.15	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	41.46	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.810		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	441.65	K	Joback Method
tc	644.37	K	Joback Method
tf	225.88	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.33	J/molxK	441.65	Joback Method
cpg	198.04	J/molxK	475.44	Joback Method
cpg	206.31	J/molxK	509.22	Joback Method
cpg	214.14	J/molxK	543.01	Joback Method
cpg	221.55	J/molxK	576.80	Joback Method
cpg	228.55	J/molxK	610.58	Joback Method
cpg	235.16	J/molxK	644.37	Joback Method
dvisc	0.0082291	Paxs	225.88	Joback Method

dvisc	0.0034166	Paxs	261.84	Joback Method
dvisc	0.0017540	Paxs	297.80	Joback Method
dvisc	0.0010396	Paxs	333.76	Joback Method
dvisc	0.0006822	Paxs	369.73	Joback Method
dvisc	0.0004824	Paxs	405.69	Joback Method
dvisc	0.0003609	Paxs	441.65	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=R630365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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