

5-Nonanone, 4,6-dichloro (RS, SR)

Inchi:	InChI=1S/C9H16Cl2O/c1-3-5-7(10)9(12)8(11)6-4-2/h7-8H,3-6H2,1-2H3
InchiKey:	WLHRBHKGHYVXJK-UHFFFAOYSA-N
Formula:	C9H16Cl2O
SMILES:	CCCC(Cl)C(=O)C(Cl)CCC
Mol. weight [g/mol]:	211.13

Physical Properties

Property code	Value	Unit	Source
gf	-132.76	kJ/mol	Joback Method
hf	-383.71	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	50.37	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.370		Crippen Method
mcvol	163.720	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
tb	533.17	K	Joback Method
tc	725.90	K	Joback Method
tf	270.96	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.23	J/molxK	533.17	Joback Method
cpg	415.29	J/molxK	693.78	Joback Method
cpg	404.71	J/molxK	661.66	Joback Method
cpg	393.53	J/molxK	629.54	Joback Method
cpg	381.74	J/molxK	597.41	Joback Method
cpg	369.31	J/molxK	565.29	Joback Method
cpg	425.29	J/molxK	725.90	Joback Method
dvisc	0.0002562	Paxs	533.17	Joback Method

dvisc	0.0003476	Paxs	489.47	Joback Method
dvisc	0.0005008	Paxs	445.77	Joback Method
dvisc	0.0007809	Paxs	402.07	Joback Method
dvisc	0.0013572	Paxs	358.36	Joback Method
dvisc	0.0027503	Paxs	314.66	Joback Method
dvisc	0.0069990	Paxs	270.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630612&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
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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