

1-Nonene, 1,1,9-trichloro-

Other names:	1,1,9-Trichloro-1-nonene
Inchi:	InChI=1S/C9H15Cl3/c10-8-6-4-2-1-3-5-7-9(11)12/h7H,1-6,8H2
InchiKey:	OASWFWUZCDHORK-UHFFFAOYSA-N
Formula:	C9H15Cl3
SMILES:	C1CCCCCCCC=C(Cl)Cl
Mol. weight [g/mol]:	229.57
CAS:	3930-10-7

Physical Properties

Property code	Value	Unit	Source
gf	60.78	kJ/mol	Joback Method
hf	-168.88	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	48.82	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.885		Crippen Method
mcvol	170.090	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
tb	521.65	K	Joback Method
tc	714.28	K	Joback Method
tf	261.91	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.12	J/mol×K	521.65	Joback Method
cpg	358.61	J/mol×K	553.76	Joback Method
cpg	370.43	J/mol×K	585.86	Joback Method
cpg	381.60	J/mol×K	617.97	Joback Method
cpg	392.17	J/mol×K	650.07	Joback Method
cpg	402.17	J/mol×K	682.18	Joback Method
cpg	411.63	J/mol×K	714.28	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3930107&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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