

1,1,1,9-Tetrachlorononane

Inchi:	InChI=1S/C9H16Cl4/c10-8-6-4-2-1-3-5-7-9(11,12)13/h1-8H2
InchiKey:	PVWUJBDIDCVQCR-UHFFFAOYSA-N
Formula:	C9H16Cl4
SMILES:	C1CCCCCCCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	266.04
CAS:	1561-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-19.98	kJ/mol	Joback Method
hf	-300.80	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	51.87	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	5.326		Crippen Method
mvol	186.630	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
tb	551.81	K	Joback Method
tc	748.78	K	Joback Method
tf	313.29	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.37	J/molxK	551.81	Joback Method
cpg	408.24	J/molxK	584.64	Joback Method
cpg	420.32	J/molxK	617.47	Joback Method
cpg	431.67	J/molxK	650.30	Joback Method
cpg	442.33	J/molxK	683.12	Joback Method
cpg	452.34	J/molxK	715.95	Joback Method
cpg	461.74	J/molxK	748.78	Joback Method
dvisc	0.0019165	Paxs	353.04	Joback Method
dvisc	0.0040529	Paxs	313.29	Joback Method

dvisc	0.0010546	Paxs	392.80	Joback Method
dvisc	0.0006477	Paxs	432.55	Joback Method
dvisc	0.0004318	Paxs	472.30	Joback Method
dvisc	0.0003066	Paxs	512.06	Joback Method
dvisc	0.0002287	Paxs	551.81	Joback Method
hvapt	78.00	kJ/mol	368.50	NIST Webbook
hvapt	89.00	kJ/mol	318.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1561484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvapt:	Enthalpy of vaporization at a given temperature
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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