

1-Heptene, 1,1,7-trichloro-

Other names:	1,1,7-Trichloro-1-heptene
Inchi:	InChI=1S/C7H11Cl3/c8-6-4-2-1-3-5-7(9)10/h5H,1-4,6H2
InchiKey:	PSSICVWETCAXGQ-UHFFFAOYSA-N
Formula:	C7H11Cl3
SMILES:	C1CCCCC=C(Cl)Cl
Mol. weight [g/mol]:	201.52
CAS:	3993-94-0

Physical Properties

Property code	Value	Unit	Source
gf	43.94	kJ/mol	Joback Method
hf	-127.60	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	4.105		Crippen Method
mcvol	141.910	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	475.89	K	Joback Method
tc	673.45	K	Joback Method
tf	239.37	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.55	J/molxK	475.89	Joback Method
cpg	271.10	J/molxK	508.82	Joback Method
cpg	281.05	J/molxK	541.74	Joback Method
cpg	290.42	J/molxK	574.67	Joback Method
cpg	299.26	J/molxK	607.59	Joback Method
cpg	307.59	J/molxK	640.52	Joback Method
cpg	315.45	J/molxK	673.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3993940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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