

1-Propene, 3-chloro-1,1,2,3,3-pentafluoro-

Other names:	Propene, 3-chloropentafluoro- Perfluoroallyl chloride 3-Chloropentafluoropropene 3-Chloro-1,1,2,3,3-pentafluoropropene
Inchi:	InChI=1S/C3CIF5/c4-3(8,9)1(5)2(6)7
InchiKey:	IJTAKAGEJXIJPQ-UHFFFAOYSA-N
Formula:	C3CIF5
SMILES:	FC(F)=C(F)C(F)(F)Cl
Mol. weight [g/mol]:	166.48
CAS:	79-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-945.64	kJ/mol	Joback Method
hf	-1012.65	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	21.39	kJ/mol	Joback Method
ie	10.79	eV	NIST Webbook
log10ws	-2.94		Crippen Method
logp	2.896		Crippen Method
mcvol	69.920	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	302.51	K	Joback Method
tc	453.20	K	Joback Method
tf	125.86	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.95	J/molxK	302.51	Joback Method
cpg	121.95	J/molxK	327.62	Joback Method
cpg	127.54	J/molxK	352.74	Joback Method
cpg	132.75	J/molxK	377.85	Joback Method

cpg	137.58	J/mol×K	402.97	Joback Method
cpg	142.07	J/mol×K	428.08	Joback Method
cpg	146.22	J/mol×K	453.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79470&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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