

Propane, 1,2,3-trichloro-1,1,2,3,3-pentafluoro-

Other names:	Propane, 1,2,3-trichloropentafluoro- 1,2,3-Trichloropentafluoropropane 1,1,2,3,3-Pentafluoro-1,2,3-trichloro propane
Inchi:	InChI=1S/C3Cl3F5/c4-1(7,2(5,8)9)3(6,10)11
InchiKey:	AIDLQDHQDQZVQM-UHFFFAOYSA-N
Formula:	C3Cl3F5
SMILES:	FC(F)(Cl)C(F)(Cl)C(F)(F)Cl
Mol. weight [g/mol]:	237.38
CAS:	76-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-1026.94	kJ/mol	Joback Method
hf	-1159.27	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	27.45	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.554		Crippen Method
mcvol	98.700	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	346.80	K	NIST Webbook
tc	542.98	K	Joback Method
tf	223.54	K	Joback Method
vc	0.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.61	J/mol×K	366.99	Joback Method
cpg	184.40	J/mol×K	396.32	Joback Method
cpg	191.42	J/mol×K	425.65	Joback Method
cpg	197.72	J/mol×K	454.99	Joback Method
cpg	203.33	J/mol×K	484.32	Joback Method
cpg	208.31	J/mol×K	513.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76175&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
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
mccvol:	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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