

Propane, 1,1,1,2,2-pentachloro-3,3,3-trifluoro-

Other names:	1,1,1-Trifluoro-2,2,3,3,3-pentachloro propane
Inchi:	InChI=1S/C3Cl5F3/c4-1(5,2(6,7)8)3(9,10)11
InchiKey:	GKXWTRSVUPXQMM-UHFFFAOYSA-N
Formula:	C3Cl5F3
SMILES:	FC(F)(F)C(Cl)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	270.29
CAS:	1652-89-7

Physical Properties

Property code	Value	Unit	Source
gf	-661.18	kJ/mol	Joback Method
hf	-798.53	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.093		Crippen Method
mcvol	119.640	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	443.31	K	Joback Method
tc	656.78	K	Joback Method
tf	282.20	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.48	J/mol×K	443.31	Joback Method
cpg	210.06	J/mol×K	478.89	Joback Method
cpg	215.71	J/mol×K	514.47	Joback Method
cpg	220.49	J/mol×K	550.04	Joback Method
cpg	224.49	J/mol×K	585.62	Joback Method
cpg	227.79	J/mol×K	621.20	Joback Method
cpg	230.48	J/mol×K	656.78	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=C1652897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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