

Propane, 1,3-dichloro-1,1,2,2,3-pentafluoro-

Other names:	1,3-dichloro-1,1,2,2,3-pentafluoropropane
Inchi:	InChI=1S/C3HCl2F5/c4-1(6)2(7,8)3(5,9)10/h1H
InchiKey:	UJIGKESMIPTWJH-UHFFFAOYSA-N
Formula:	C3HCl2F5
SMILES:	FC(Cl)C(F)(F)C(F)(F)Cl
Mol. weight [g/mol]:	202.94
CAS:	507-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-1020.29	kJ/mol	Joback Method
hf	-1140.06	kJ/mol	Joback Method
hfus	8.97	kJ/mol	Joback Method
hvap	23.98	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.988		Crippen Method
mcvol	86.460	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	325.20 ± 3.00	K	NIST Webbook
tc	492.17	K	Joback Method
tf	176.20	K	Joback Method
vc	0.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.04	J/mol×K	332.35	Joback Method
cpg	159.36	J/mol×K	358.99	Joback Method
cpg	166.13	J/mol×K	385.62	Joback Method
cpg	172.39	J/mol×K	412.26	Joback Method
cpg	178.17	J/mol×K	438.89	Joback Method
cpg	183.48	J/mol×K	465.53	Joback Method
cpg	188.34	J/mol×K	492.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55061e+01
Coeff. B	-3.19094e+03
Coeff. C	-3.21250e+01
Temperature range (K), min.	241.80
Temperature range (K), max.	347.84

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507551&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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