

Propane, 3-chloro-1,1,1-trifluoro-

Other names:	1,1,1-Trifluoro-3-chloropropane 1-Chloro-3,3,3-trifluoropropane 3,3,3-Trifluoro-1-chloropropane 3-Chloro-1,1,1-trifluoropropane CF ₃ CH ₂ CH ₂ Cl Freon 253
Inchi:	InChI=1S/C3H4ClF3/c4-2-1-3(5,6)7/h1-2H2
InchiKey:	ZPIFKCVYZBVZIV-UHFFFAOYSA-N
Formula:	C ₃ H ₄ ClF ₃
SMILES:	FC(F)(F)CCCl
Mol. weight [g/mol]:	132.51
CAS:	460-35-5

Physical Properties

Property code	Value	Unit	Source
chl	-1504.20 ± 0.92	kJ/mol	NIST Webbook
gf	-619.14	kJ/mol	Joback Method
hf	-718.07	kJ/mol	Joback Method
hfl	-799.31 ± 0.92	kJ/mol	NIST Webbook
hfus	9.55	kJ/mol	Joback Method
hvap	22.91	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	2.178		Crippen Method
mcvol	70.680	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
sl	271.67	J/mol×K	NIST Webbook
sl	271.67	J/mol×K	NIST Webbook
tb	319.00	K	NIST Webbook
tc	453.65	K	Joback Method
tf	157.68	K	Joback Method
tt	179.32 ± 0.02	K	NIST Webbook
tt	179.40 ± 0.02	K	NIST Webbook
vc	0.295	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.12	J/mol×K	453.65	Joback Method
cpg	112.93	J/mol×K	300.05	Joback Method
cpg	142.20	J/mol×K	428.05	Joback Method
cpg	136.98	J/mol×K	402.45	Joback Method
cpg	131.46	J/mol×K	376.85	Joback Method
cpg	125.62	J/mol×K	351.25	Joback Method
cpg	119.45	J/mol×K	325.65	Joback Method
cpl	171.08	J/mol×K	298.15	NIST Webbook
cpl	171.08	J/mol×K	298.15	NIST Webbook
hfust	5.05	kJ/mol	179.30	NIST Webbook
hfust	4.49	kJ/mol	169.80	NIST Webbook
hfust	5.31	kJ/mol	179.40	NIST Webbook
hvapt	33.70	kJ/mol	321.00	NIST Webbook
hvapt	29.90	kJ/mol	306.00	NIST Webbook
sfust	26.44	J/mol×K	169.80	NIST Webbook
sfust	28.20	J/mol×K	179.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38810e+01
Coeff. B	-2.47417e+03
Coeff. C	-5.18870e+01
Temperature range (K), min.	233.90
Temperature range (K), max.	340.61

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C460355&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.cheméo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor pressure
sfust: Entropy of fusion at a given temperature
sl: Liquid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume

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