Ethane, 1,1,2-trichloro-1-fluoro-

Other names: 1,1,2-Trichloro-1-fluoroethane
1,1,2-trichlorofluoroethane
Inchi: InChI=1S/C2H2Cl3F/c3-1-2(4,5)6/h1H2
InchiKey: ZKVMMSGRDBQIOQ-UHFFFAOYSA-N
Formula: C2H2Cl3F
SMILES: FC(Cl)(Cl)CCl
Mol. weight [g/mol]: 151.40
CAS: 811-95-0

Physical Properties

Property code	Value	Unit	Source
gf	-261.80	kJ/mol	Joback Method
hf	-336.69	kJ/mol	Joback Method
hfus	9.19	kJ/mol	Joback Method
hvap	31.09	kJ/mol	Joback Method
log10ws	-3.04		Aqueous Solubility Prediction Method
logp	2.326		Crippen Method
mcvol	77.530	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	361.00	K	NIST Webbook
tc	547.91	K	Joback Method
tf	205.07	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.11	J/mol×K	353.49	Joback Method
cpg	114.05	J/mol×K	385.89	Joback Method
cpg	118.58	J/mol×K	418.30	Joback Method
cpg	122.71	J/mol×K	450.70	Joback Method
cpg	126.47	J/mol×K	483.10	Joback Method
cpg	129.89	J/mol×K	515.51	Joback Method

cpg	132.99	J/mol×K	547.91	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38401e+01
Coeff. B	-2.70079e+03
Coeff. C	-6.81280e+01
Temperature range (K), min.	267.41
Temperature range (K), max.	385.01

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C811950&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/ci990307l

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

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