1-chloro-1,2,2-trifluoroethane

Inchi: InChI=1S/C2H2ClF3/c3-1(4)2(5)6/h1-2H
InchiKey: FWAQVJAOVDYHAF-UHFFFAOYSA-N
Formula: C2H2ClF3
SMILES: FC(F)C(F)Cl
Mol. weight [g/mol]: 118.48
CAS: 431-07-2

Physical Properties

Property code	Value	Unit	Source
af	0.2896		Cheméo Relay (1.0)
gf	-635.28	kJ/mol	Joback Method
hf	-722.56	kJ/mol	Cheméo Relay (1.0)
hfus	7.33	kJ/mol	Joback Method
ie	12.01	eV	Cheméo Relay (1.0)
logp	1.786		Crippen Method
mcvol	56.590	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	293.41	K	Cheméo Relay (1.0)
tc	463.43	K	Cheméo Relay (1.0)
tf	200.01	K	Cheméo Relay (1.0)
vc	0.243	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.37	J/mol×K	279.52	Joback Method
cpg	90.43	J/mol×K	304.38	Joback Method
cpg	94.34	J/mol×K	329.24	Joback Method
cpg	98.09	J/mol×K	354.10	Joback Method
cpg	101.69	J/mol×K	378.96	Joback Method
cpg	105.14	J/mol×K	403.82	Joback Method
cpg	108.46	J/mol×K	428.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57537e+01
Coeff. B	-2.93521e+03
Coeff. C	-2.41870e+01
Temperature range (K), min.	213.97
Temperature range (K), max.	308.41

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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