1-chloro-2,2-difluoropropane

Inchi: InChI=1S/C3H5ClF2/c1-3(5,6)2-4/h2H2,1H3
InchiKey: OOXYGJSMTMPTFW-UHFFFAOYSA-N
Formula: C3H5ClF2
SMILES: CC(F)(F)CCl
Mol. weight [g/mol]: 114.52
CAS: 420-99-5

Physical Properties

Property code	Value	Unit	Source
af	0.2634		Cheméo Relay (1.0)
gf	-424.33	kJ/mol	Joback Method
hf	-552.23	kJ/mol	Cheméo Relay (1.0)
hfus	6.47	kJ/mol	Joback Method
ie	10.99	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.880		Crippen Method
mcvol	68.910	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	324.69	K	Cheméo Relay (1.0)
tc	493.83	K	Cheméo Relay (1.0)
tf	194.94	K	Cheméo Relay (1.0)
vc	0.260	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.82	J/mol×K	300.78	Joback Method
cpg	111.62	J/mol×K	327.94	Joback Method
cpg	118.06	J/mol×K	355.09	Joback Method
cpg	124.14	J/mol×K	382.25	Joback Method
cpg	129.88	J/mol×K	409.41	Joback Method
cpg	135.29	J/mol×K	436.56	Joback Method
cpg	140.39	J/mol×K	463.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64758e+01
Coeff. B	-3.40185e+03
Coeff. C	-3.23760e+01
Temperature range (K), min.	242.52
Temperature range (K), max.	337.08

Sources

Cheméo Relay (1.0, beta):

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):

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
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