Acetic acid, trifluoro-, 2,2,2-trifluoroethyl ester

Other names:	2,2,2-Trifluoroethyl trifluoroacetate
	CF3C(O)OCH2CF3
	Trifluoroacetic acid trifluoroethyl ester
Inchi:	InChI=1S/C4H2F6O2/c5-3(6,7)1-12-2(11)4(8,9)10/h1H2
InchiKey:	ZKUJOCJJXCPCFS-UHFFFAOYSA-N
Formula:	C4H2F6O2
SMILES:	O=C(OCC(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	196.05
CAS:	407-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-1414.30	kJ/mol	Joback Method
hf	-1564.85	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	26.16	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.654		Crippen Method
mcvol	85.280	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	328.00	K	NIST Webbook
tb	328.20	K	NIST Webbook
tc	502.85	K	Joback Method
tf	215.38	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.39	J/mol×K	356.37	Joback Method
cpg	188.79	J/mol×K	380.78	Joback Method
cpg	195.79	J/mol×K	405.20	Joback Method
cpg	202.40	J/mol×K	429.61	Joback Method
cpg	208.64	J/mol×K	454.03	Joback Method

cpg	214.53	J/mol×K	478.44	Joback Method
cpg	220.06	J/mol×K	502.85	Joback Method
hvapt	31.80	kJ/mol	330.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62909e+01
Coeff. B	-3.82920e+03
Temperature range (K), min.	239.27
Temperature range (K), max.	348.76

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C407385&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1785.mol

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume