

2,2,2-Trifluoroethyl trifluoroacetate

Other names:	Acetic acid, trifluoro-, 2,2,2-trifluoroethyl ester 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
hf	-1645.09	kJ/mol	Cheméo Relay (1.0)
hfus	12.55	kJ/mol	Joback Method
hvap	37.63	kJ/mol	Cheméo Relay (1.0)
ie	11.95	eV	Cheméo Relay (1.0)
logp	1.654		Crippen Method
mcvol	85.280	ml/mol	McGowan Method
tb	329.02	K	Cheméo Relay (1.0)

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

Correlations

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

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C407385&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1785.mol

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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