

Acetic acid, trifluoro-, ethyl ester

Other names:	CF ₃ COOC ₂ H ₅ Ethyl ester of Trifluoroacetic acid Ethyl trifluoroacetate Ethyl trifluoroethanoate Trifluoroacetic acid, ethyl ester acetic acid, 2,2,2-trifluoro-, ethyl ester ethyl 2,2,2-trifluoroacetate ethyl perfluoroacetate trifluoroacetic acid ethyl ester
Inchi:	InChI=1S/C ₄ H ₅ F ₃ O ₂ /c1-2-9-3(8)4(5,6)7/h2H2,1H3
InchiKey:	STSCVKRWJPWALQ-UHFFFAOYSA-N
Formula:	C ₄ H ₅ F ₃ O ₂
SMILES:	CCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	142.08
CAS:	383-63-1

Physical Properties

Property code	Value	Unit	Source
affp	758.80	kJ/mol	NIST Webbook
basg	727.90	kJ/mol	NIST Webbook
gf	-832.71	kJ/mol	Joback Method
hf	-967.77	kJ/mol	Joback Method
hfus	10.73	kJ/mol	Joback Method
hvap	29.91	kJ/mol	Joback Method
ie	11.60	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	1.112		Crippen Method
mcvol	79.970	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	473.80		NIST Webbook
rinpol	474.00		NIST Webbook
tb	335.65	K	Isobaric vapor-liquid equilibrium of trifluoroacetic acid + water, trifluoroacetic acid + ethyl trifluoroacetate and ethyl trifluoroacetate + ethanol binary mixtures

tb	334.00 ± 1.00	K	NIST Webbook
tb	334.20	K	NIST Webbook
tc	523.58	K	Joback Method
tf	211.19	K	Joback Method
vc	0.327	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.68	J/mol×K	361.79	Joback Method
cpg	162.85	J/mol×K	388.75	Joback Method
cpg	169.70	J/mol×K	415.72	Joback Method
cpg	176.25	J/mol×K	442.68	Joback Method
cpg	182.51	J/mol×K	469.65	Joback Method
cpg	188.47	J/mol×K	496.61	Joback Method
cpg	194.16	J/mol×K	523.58	Joback Method
hvapt	34.70	kJ/mol	335.00	NIST Webbook
rfi	1.30860		293.15	Density, viscosity, and saturated vapor pressure of ethyl trifluoroacetate

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.70839e+01
Coeff. B	-4.16538e+03
Temperature range (K), min.	247.99
Temperature range (K), max.	353.82

Sources

Joback Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C383631&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

Isobaric vapor-liquid equilibrium of trifluoroacetic acid + water, trifluoroacetic acid + ethanol, trifluoroacetate + ethanol binary mixtures: <https://www.doi.org/10.1016/j.fluid.2015.08.012>

Enthalpy of fusion and saturated vapor pressure of ethyl trifluoroacetate: <https://www.doi.org/10.1016/j.jct.2015.02.022>

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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