Trifluoroacetic acid, propyl ester

Other names:	Acetic acid, trifluoro-, propyl ester
	Propyl trifluoroacetate
	CF3CO2(n-C3H7)
Inchi:	InChI=1S/C5H7F3O2/c1-2-3-10-4(9)5(6,7)8/h2-3H2,1H3
InchiKey:	CDXJNCAVPFGVNL-UHFFFAOYSA-N
Formula:	C5H7F3O2
SMILES:	CCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	156.10

Physical Properties

Property code	Value	Unit	Source
affp	763.90	kJ/mol	NIST Webbook
basg	732.90	kJ/mol	NIST Webbook
hf	-1040.71	kJ/mol	Cheméo Relay (1.0)
hfus	13.32	kJ/mol	Joback Method
hvap	34.17	kJ/mol	Cheméo Relay (1.0)
ie	11.15	eV	Cheméo Relay (1.0)
log10ws	-0.76		Cheméo Relay (1.0)
logp	1.502		Crippen Method
mcvol	94.060	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	559.00		NIST Webbook
rinpol	558.60		NIST Webbook
rinpol	569.60		NIST Webbook
tb	360.42	K	Cheméo Relay (1.0)
tc	469.97	K	Cheméo Relay (1.0)
tf	191.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.04	J/mol×K	384.67	Joback Method
cpg	198.49	J/mol×K	411.62	Joback Method
cpg	206.57	J/mol×K	438.57	Joback Method

cpg	214.30	J/mol×K	465.52	Joback Method
cpg	221.68	J/mol×K	492.47	Joback Method
cpg	228.73	J/mol×K	519.42	Joback Method
cpg	235.45	J/mol×K	546.37	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C383664&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point