1-Pentanol, trifluoroacetate

Other names:	Pentyl trifluoroacetate
	Pentyl 2,2,2-trifluoroacetate
	Trifluoroacetic acid, n-pentyl ester
	Acetic acid, trifluoro-, pentyl ester
	Trifluoroacetic acid, pentyl ester
Inchi:	InChI=1S/C7H11F3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h2-5H2,1H3
InchiKey:	XJVUVRKPEBTMEC-UHFFFAOYSA-N
Formula:	C7H11F3O2
SMILES:	CCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	184.16
CAS:	327-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-807.45	kJ/mol	Joback Method
hf	-1029.69	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	36.59	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.282		Crippen Method
mcvol	122.240	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	772.00		NIST Webbook
rinpol	788.80		NIST Webbook
rinpol	776.20		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	752.10		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	752.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	877.00		NIST Webbook
tb	396.15 ± 1.50	K	NIST Webbook
tc	591.25	K	Joback Method
tf	245.00	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.87	J/mol×K	430.43	Joback Method
cpg	276.54	J/mol×K	457.23	Joback Method
cpg	286.76	J/mol×K	484.04	Joback Method
cpg	296.54	J/mol×K	510.84	Joback Method
cpg	305.89	J/mol×K	537.64	Joback Method
cpg	314.82	J/mol×K	564.45	Joback Method
cpg	323.34	J/mol×K	591.25	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C327708&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume