Isopropyl trifluoroacetate

Other names: Acetic acid, trifluoro-, 1-methylethyl ester
Trifluoroacetic acid, isopropyl ester
Inchi: InChI=1S/C5H7F3O2/c1-3(2)10-4(9)5(6,7)8/h3H,1-2H3
InchiKey: ASAXRKSDVDALDT-UHFFFAOYSA-N
Formula: C5H7F3O2
SMILES: CC(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 156.10
CAS: 400-38-4

Physical Properties

Property code	Value	Unit	Source
gf	-826.73	kJ/mol	Joback Method
hf	-993.69	kJ/mol	Joback Method
hfus	9.80	kJ/mol	Joback Method
hvap	31.75	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.500		Crippen Method
mcvol	94.060	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	528.80		NIST Webbook
rinpol	528.80		NIST Webbook
tb	359.00	K	NIST Webbook
tb	346.60	K	NIST Webbook
tc	549.62	K	Joback Method
tf	207.46	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.00	J/mol×K	384.23	Joback Method
cpg	198.72	J/mol×K	411.79	Joback Method
cpg	207.06	J/mol×K	439.36	Joback Method
cpg	215.02	J/mol×K	466.92	Joback Method

cpg	222.62	J/mol×K	494.49	Joback Method
cpg	229.86	J/mol×K	522.05	Joback Method
cpg	236.76	J/mol×K	549.62	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1790.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C400384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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