2,2,2-Trifluoroethyl acetate

Inchi: InChI=1S/C5H7F3O2/c1-2-10-4(9)3-5(6,7)8/h2-3H2,1H3
InchiKey: FMDMKDPUFQNVSH-UHFFFAOYSA-N
Formula: C5H7F3O2
SMILES: CCOC(=O)CC(F)(F)F
Mol. weight [g/mol]: 156.10

Physical Properties

Property code	Value	Unit	Source
gf	-824.29	kJ/mol	Joback Method
hf	-988.41	kJ/mol	Joback Method
hfus	13.32	kJ/mol	Joback Method
hvap	32.13	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.502		Crippen Method
mcvol	94.060	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	527.00		NIST Webbook
rinpol	527.00		NIST Webbook
tb	384.67	K	Joback Method
tc	546.37	K	Joback Method
tf	222.46	K	Joback Method
vc	0.383	m3/kmol	Joback Method

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

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=R595430&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume