2-Methoxyethyl 2,2,2-trifluoroacetate

Other names: 2-Methoxyethanol, trifluoroacetate
Inchi: InChI=1S/C5H7F3O3/c1-10-2-3-11-4(9)5(6,7)8/h2-3H2,1H3
InchiKey: CZDCICPBYIRPFA-UHFFFAOYSA-N
Formula: C5H7F3O3
SMILES: COCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 172.10

Physical Properties

Property code	Value	Unit	Source
gf	-929.29	kJ/mol	Joback Method
hf	-1120.63	kJ/mol	Joback Method
hfus	14.51	kJ/mol	Joback Method
hvap	34.54	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.738		Crippen Method
mcvol	99.930	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	739.00		NIST Webbook
tb	407.09	K	Joback Method
tc	569.32	K	Joback Method
tf	244.69	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.56	J/mol×K	407.09	Joback Method
cpg	219.76	J/mol×K	434.13	Joback Method
cpg	227.66	J/mol×K	461.17	Joback Method
cpg	235.26	J/mol×K	488.21	Joback Method
cpg	242.56	J/mol×K	515.24	Joback Method
cpg	249.58	J/mol×K	542.28	Joback Method
cpg	256.30	J/mol×K	569.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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