2-Hydroxyethyl 2,2,2-trifluoroacetate

Other names: Ethylene glycol, mono(trifluoroacetate)
Inchi: InChI=1S/C4H5F3O3/c5-4(6,7)3(9)10-2-1-8/h8H,1-2H2
InchiKey: MGECQCPJQHINMP-UHFFFAOYSA-N
Formula: C4H5F3O3
SMILES: O=C(OCCO)C(F)(F)F
Mol. weight [g/mol]: 158.08

Physical Properties

Property code	Value	Unit	Source
gf	-969.53	kJ/mol	Joback Method
hf	-1120.00	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	46.59	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.084		Crippen Method
mcvol	85.840	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	768.50		NIST Webbook
tb	453.97	K	Joback Method
tc	612.86	K	Joback Method
tf	272.01	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.28	J/mol×K	453.97	Joback Method
cpg	200.62	J/mol×K	480.45	Joback Method
cpg	206.66	J/mol×K	506.93	Joback Method
cpg	212.42	J/mol×K	533.41	Joback Method
cpg	217.89	J/mol×K	559.90	Joback Method
cpg	223.08	J/mol×K	586.38	Joback Method
cpg	228.01	J/mol×K	612.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351921&Units=SI

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