1,1-Ethanediol, 2,2,2-trifluoro-1-(4-methoxyphenyl)-

Inchi: InChI=1S/C9H9F3O3/c1-15-7-4-2-6(3-5-7)8(13,14)9(10,11)12/h2-5,13-14H,1H3
InchiKey: OVYVMUARAPGOIN-UHFFFAOYSA-N
Formula: C9H9F3O3
SMILES: COc1ccc(C(O)(O)C(F)(F)F)cc1
Mol. weight [g/mol]: 222.16
CAS: 110374-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-829.71	kJ/mol	Joback Method
hf	-1046.54	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.395		Crippen Method
mcvol	136.830	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	635.11	K	Joback Method
tc	815.64	K	Joback Method
tf	380.61	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.60	J/mol×K	635.11	Joback Method
cpg	377.30	J/mol×K	665.20	Joback Method
cpg	385.40	J/mol×K	695.29	Joback Method
cpg	392.94	J/mol×K	725.38	Joback Method
cpg	399.96	J/mol×K	755.46	Joback Method
cpg	406.49	J/mol×K	785.55	Joback Method
cpg	412.56	J/mol×K	815.64	Joback Method

Sources

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=C110374828&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume