Benzeneethanol, 2,2,2-trifluoro-1-(4-fluorophenyl)

Inchi: InChI=1S/C8H6F4O/c9-6-3-1-5(2-4-6)7(13)8(10,11)12/h1-4,7,13H

InchiKey: BDQHSIMDNYIOMB-UHFFFAOYSA-N

Formula: C8H6F4O

SMILES: OC(c1ccc(F)cc1)C(F)(F)F

Mol. weight [g/mol]: 194.13

Physical Properties

Property code	Value	Unit	Source
gf	-796.40	kJ/mol	Joback Method
hf	-934.09	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.421		Crippen Method
mcvol	112.770	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1035.00		NIST Webbook
tb	499.69	K	Joback Method
tc	676.46	K	Joback Method
tf	269.46	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.44	J/mol×K	499.69	Joback Method
cpg	269.94	J/mol×K	529.15	Joback Method
cpg	278.84	J/mol×K	558.61	Joback Method
cpg	287.17	J/mol×K	588.07	Joback Method
cpg	294.94	J/mol×K	617.54	Joback Method
cpg	302.21	J/mol×K	647.00	Joback Method
cpg	308.98	J/mol×K	676.46	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=R515201&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