Benzamide, 2,3,4-trifluoro-N-ethyl-

Inchi: InChI=1S/C9H8F3NO/c1-2-13-9(14)5-3-4-6(10)8(12)7(5)11/h3-4H,2H2,1H3,(H,13,14)
InchiKey: XAEIMVWLTDXKIM-UHFFFAOYSA-N
Formula: C9H8F3NO
SMILES: CCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 203.16

Physical Properties

Property code	Value	Unit	Source
gf	-515.54	kJ/mol	Joback Method
hf	-674.41	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	50.62	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	1.854		Crippen Method
mcvol	130.770	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
tb	548.79	K	Joback Method
tc	740.48	K	Joback Method
tf	359.53	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.86	J/mol×K	548.79	Joback Method
cpg	312.20	J/mol×K	580.74	Joback Method
cpg	322.00	J/mol×K	612.69	Joback Method
cpg	331.29	J/mol×K	644.64	Joback Method
cpg	340.06	J/mol×K	676.58	Joback Method
cpg	348.34	J/mol×K	708.53	Joback Method
cpg	356.13	J/mol×K	740.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407257&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