Benzamide, 2-(trifluoromethyl)-N-ethyl-

Inchi: InChI=1S/C10H10F3NO/c1-2-14-9(15)7-5-3-4-6-8(7)10(11,12)13/h3-6H,2H2,1H3,(H,14,1
InchiKey: GTHIVDIEQVLQIQ-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: CCN=C(O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 217.19

Physical Properties

Property code	Value	Unit	Source
hf	-701.55	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	3.030		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	623.18	K	Joback Method
tc	819.18	K	Joback Method

Sources

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=U407183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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