

Benzamide, 2,5-di(trifluoromethyl)-N-ethyl-

Inchi:	InChI=1S/C11H9F6NO/c1-2-18-9(19)7-5-6(10(12,13)14)3-4-8(7)11(15,16)17/h3-5H,2H2,
InchiKey:	OXYVDPDJRWLQCT-UHFFFAOYSA-N
Formula:	C11H9F6NO
SMILES:	CCN=C(O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	285.19

Physical Properties

Property code	Value	Unit	Source
hf	-1330.74	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.049		Crippen Method
mcvol	164.260	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinsol	1322.00		NIST Webbook
tb	645.62	K	Joback Method
tc	827.25	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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