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

Inchi: InChI=1S/C12H11F6NO/c1-2-5-19-10(20)8-6-7(11(13,14)15)3-4-9(8)12(16,17)18/h3-4,6H

InchiKey: ORFURDFVALKZCW-UHFFFAOYSA-N

Formula: C12H11F6NO

SMILES: CCCN=C(O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 299.21

Physical Properties

Property code	Value	Unit	Source
hf	-1351.38	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.439		Crippen Method
mcvol	178.350	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1396.00		NIST Webbook
tb	668.50	K	Joback Method
tc	849.11	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=U407916&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