

Benzamide, N-(3-chlorophenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C13H7ClF3NO/c14-7-2-1-3-8(6-7)18-13(19)9-4-5-10(15)12(17)11(9)16/h1-6H,
InchiKey: CXWYWCNYBSGLEK-UHFFFAOYSA-N
Formula: C13H7ClF3NO
SMILES: OC(=Nc1cccc(Cl)c1)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 285.65

Physical Properties

Property code	Value	Unit	Source
hf	-568.34	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.394		Crippen Method
mcvol	175.610	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	774.10	K	Joback Method
tc	992.71	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307176&Units=SI>

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

Latest version available from:

<https://www.cheméo.com/cid/90-888-7/Benzamide-N-3-chlorophenyl-2-3-4-trifluoro.pdf>

Generated by Cheméo on 2024-04-27 08:02:54.061700757 +0000 UTC m=+16494222.982278072.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.