3,5-Bis(trifluoromethyl)pyrazol

Other names:	3,3-Bis(trifluoromethyl)pyrazol
	3,5-bis(trifluoromethyl)pyrazole
Inchi:	InChI=1S/C5H2F6N2/c6-4(7,8)2-1-3(13-12-2)5(9,10)11/h1H,(H,12,13)
InchiKey:	NGDDUAYSWPUSLX-UHFFFAOYSA-N
Formula:	C5H2F6N2
SMILES:	FC(F)(F)c1cc(C(F)(F)F)[nH]n1
Mol. weight [g/mol]:	204.07
CAS:	14704-41-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	1.965		Crippen Method
mcvol	92.430	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	69.00 ± 0.60	kJ/mol	266.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14704417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume