4-Methoxybenzaldehyde, PFBO # 1

Inchi: InChI=1S/C15H10F5NO2/c1-22-9-4-2-8(3-5-9)6-21-23-7-10-11(16)13(18)15(20)14(19)12

InchiKey: HDKKZKNAURGNMX-UHFFFAOYSA-N

Formula: C15H10F5NO2

SMILES: COc1ccc(C=NOCc2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 331.24

Physical Properties

Property code	Value	Unit	Source
hf	-1111.46	kJ/mol	Joback Method
hvap	61.56	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.941		Crippen Method
mcvol	200.960	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
ripol	2718.00		NIST Webbook
ripol	2718.00		NIST Webbook
tb	743.71	K	Joback Method
tc	945.89	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=R575050&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature