

3-Hydroxy-4-methoxybenzaldehyde, PFBO # 1

Inchi: InChI=1S/C15H10F5NO3/c1-23-10-3-2-7(4-9(10)22)5-21-24-6-8-11(16)13(18)15(20)14(19)
InchiKey: CHOVDYQQVWNGFN-UHFFFAOYSA-N
Formula: C15H10F5NO3
SMILES: COc1ccc(C=NOCc2c(F)c(F)c(F)c(F)c2F)cc1O
Mol. weight [g/mol]: 347.24

Physical Properties

Property code	Value	Unit	Source
hf	-1288.77	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.647		Crippen Method
mcvol	206.830	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
ripol	2724.00		NIST Webbook
ripol	2724.00		NIST Webbook
tb	824.33	K	Joback Method
tc	1035.76	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R574913&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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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