

1-(8-Bromo-2,3,6,7-tetrahydrodibenzo[1,2-b; 4,5-b']difuran-4-yl-2-aminopropane, TFA

Inchi:	InChI=1S/C15H15BrF3NO3/c1-7(20-14(21)15(17,18)19)6-10-8-2-4-23-13(8)11(16)9-3-5-
InchiKey:	YDTGXJHAFGAOCD-UHFFFAOYSA-N
Formula:	C15H15BrF3NO3
SMILES:	CC(Cc1c2c(c(Br)c3c1OCC3)OCC2)N=C(O)C(F)(F)F
Mol. weight [g/mol]:	394.18

Physical Properties

Property code	Value	Unit	Source
hf	-907.30	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.769		Crippen Method
mcvol	222.830	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2243.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	899.94	K	Joback Method
tc	1122.61	K	Joback Method

Sources

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=R640510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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