Benzamide, N-(2-piperidinylmethyl)-2,5-bis(2,2,2-trifluoroethox

Other names: Flecainide

N-(2-Piperidylmethyl)-2,5-bis(2,2,2-trifluoroethoxy)benzamide

Inchi: InChI=1S/C17H20F6N2O3/c18-16(19,20)9-27-12-4-5-14(28-10-17(21,22)23)13(7-12)15(

InchiKey: DJBNUMBKLMJRSA-UHFFFAOYSA-N

Formula: C17H20F6N2O3

SMILES: OC(=NCC1CCCCN1)c1cc(OCC(F)(F)F)ccc1OCC(F)(F)F

Mol. weight [g/mol]: 414.34

CAS: 54143-55-4

Physical Properties

Property code	Value	Unit	Source
hf	-1626.89	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.016		Crippen Method
mcvol	259.660	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	895.84	K	Joback Method
tc	1103.04	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C54143554&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

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