Benfluorex

Other names:	Ethanol, 2-[[1-methyl-2-[3-(trifluoromethyl)phenyl]ethyl]amino]-, benzoate Ethanol, 2-(«alpha»-methyl-m-trifluoromethylphenethylamino)-, benzoate N-(2-Hydroxyethyl)-«alpha»-methyl-m-trifluoromethylphenethylamine benzoate 2-(«alpha»-Methyl-m-trifluoromethylphenethylamino)ethanol benzoate Phenethylamine, N-(2-hydroxyethyl)-«alpha»-methyl-m-trifluoromethyl-, benzoate 2-[[«alpha»-Methyl-m-(trifluoromethyl)phenethyl]amino]ethanol benzoate (ester) Minolip S-780 SE-780 Benfluramate N-(2-Benzoyloxyethyl)norfenfluramine
Inchi:	InChI=1S/C19H20F3NO2/c1-14(12-15-6-5-9-17(13-15)19(20,21)22)23-10-11-25-18(24)1
InchiKey:	CJAVTWRYCDNHSM-UHFFFAOYSA-N
Formula:	C19H20F3NO2
SMILES:	CC(Cc1cccc(C(F)(F)F)c1)NCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	351.36
CAS:	23602-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-404.27	kJ/mol	Joback Method
hf	-767.59	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	74.56	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.083		Crippen Method
mcvol	253.780	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	813.06	K	Joback Method
tc	1025.30	K	Joback Method
tf	483.26	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.74	J/mol×K	813.06	Joback Method
cpg	777.13	J/mol×K	848.43	Joback Method
cpg	790.41	J/mol×K	883.81	Joback Method
cpg	802.65	J/mol×K	919.18	Joback Method
cpg	813.92	J/mol×K	954.55	Joback Method
cpg	824.29	J/mol×K	989.93	Joback Method
cpg	833.84	J/mol×K	1025.30	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=C23602780&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tf: Normal melting (fusion) point
vc: Critical Volume