Fenfluramine

Other names:	Benzeneethanamine, N-ethyl-«alpha»-methyl-3-(trifluoromethyl)- Phenethylamine, N-ethyl-«alpha»-methyl-m-(trifluoromethyl)- N-Ethyl-«alpha»-methyl-3-trifluoromethylphenethylamine 3-(Trifluoromethyl)-N-ethyl-«alpha»-methylphenethylamine 1-(meta-Trifluoromethyl-phenyl)-2 ethylaminopropane Acino Obedrex Pesos Ponderax PA Rotondin DL-Fenfluramine
Inchi:	InChI=1S/C12H16F3N/c1-3-16-9(2)7-10-5-4-6-11(8-10)12(13,14)15/h4-6,8-9,16H,3,7H2,
InchiKey:	DBGIVFWFUFKIQN-UHFFFAOYSA-N
Formula:	C12H16F3N
SMILES:	CCNC(C)Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	231.26
CAS:	458-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-341.70	kJ/mol	Joback Method
hf	-614.84	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.246		Crippen Method
mcvol	171.470	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1240.60		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1220.00		NIST Webbook

rinpol	1183.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1240.60		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1532.00		NIST Webbook
tb	549.93	K	Joback Method
tc	738.82	K	Joback Method
tf	305.79	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.52	J/mol×K	549.93	Joback Method
cpg	441.97	J/mol×K	581.41	Joback Method
cpg	456.50	J/mol×K	612.89	Joback Method
cpg	470.15	J/mol×K	644.37	Joback Method
cpg	482.98	J/mol×K	675.86	Joback Method
cpg	495.02	J/mol×K	707.34	Joback Method
cpg	506.31	J/mol×K	738.82	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C458242&Units=SI

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume