N-Methylamphetamine, N-TFA

Inchi: InChI=1S/C12H14F3NO/c1-9(8-10-6-4-3-5-7-10)16(2)11(17)12(13,14)15/h3-7,9H,8H2,1-
InchiKey: AXAFMXNUGNZMCK-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CC(Cc1ccccc1)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-439.60	kJ/mol	Joback Method
hf	-701.89	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.638		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
tb	561.09	K	Joback Method
tc	753.59	K	Joback Method
tf	323.01	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.30	J/mol×K	561.09	Joback Method
cpg	447.46	J/mol×K	593.17	Joback Method
cpg	461.60	J/mol×K	625.26	Joback Method
cpg	474.78	J/mol×K	657.34	Joback Method
cpg	487.06	J/mol×K	689.43	Joback Method
cpg	498.49	J/mol×K	721.51	Joback Method
cpg	509.13	J/mol×K	753.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412214&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume