Trifluoroacetamide, N-methyl-N-(3-methylphenyl)-

Other names: N,3-Dimethylaniline, TFA
Inchi: InChI=1S/C10H10F3NO/c1-7-4-3-5-8(6-7)14(2)9(15)10(11,12)13/h3-6H,1-2H3
InchiKey: URUJKCWKYPSNAI-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: Cc1cccc(N(C)C(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 217.19

Physical Properties

Property code	Value	Unit	Source
gf	-463.63	kJ/mol	Joback Method
hf	-666.80	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	45.83	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.520		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	520.75	K	Joback Method
tc	715.31	K	Joback Method
tf	327.99	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.28	J/mol×K	520.75	Joback Method
cpg	351.55	J/mol×K	553.18	Joback Method
cpg	363.93	J/mol×K	585.60	Joback Method
cpg	375.46	J/mol×K	618.03	Joback Method
cpg	386.19	J/mol×K	650.46	Joback Method
cpg	396.16	J/mol×K	682.89	Joback Method
cpg	405.42	J/mol×K	715.31	Joback Method

Sources

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=U328347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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