

Trifluoroacetamide, n-methyl-n-(2-methylphenyl)-

Other names:	N,2-Dimethylaniline, TFA
Inchi:	InChI=1S/C10H10F3NO/c1-7-5-3-4-6-8(7)14(2)9(15)10(11,12)13/h3-6H,1-2H3
InchiKey:	YEXXRAVVOQDXOJ-UHFFFAOYSA-N
Formula:	C10H10F3NO
SMILES:	Cc1ccccc1N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]:	217.19

Physical Properties

Property code	Value	Unit	Source
hfus	21.75	kJ/mol	Joback Method
ie	8.86	eV	Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	486.84	K	Cheméo Relay (1.0)
tc	665.36	K	Cheméo Relay (1.0)
tf	256.94	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U328346&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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

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