

Trifluoroacetamide, N-benzyl-N-methyl-

Other names:	N-Methylbenzylamine, TFA
Inchi:	InChI=1S/C10H10F3NO/c1-14(9(15)10(11,12)13)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	VGRXJRLQGWBML-UHFFFAOYSA-N
Formula:	C10H10F3NO
SMILES:	CN(Cc1ccccc1)C(=O)C(F)(F)F
Mol. weight [g/mol]:	217.19
CAS:	68464-36-8

Physical Properties

Property code	Value	Unit	Source
gf	-454.00	kJ/mol	Joback Method
hf	-655.33	kJ/mol	Joback Method
hfus	22.14	kJ/mol	Joback Method
hvap	45.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.207		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	515.77	K	Joback Method
tc	709.23	K	Joback Method
tf	315.47	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.12	J/mol×K	515.77	Joback Method
cpg	351.76	J/mol×K	548.01	Joback Method
cpg	364.45	J/mol×K	580.26	Joback Method
cpg	376.25	J/mol×K	612.50	Joback Method
cpg	387.21	J/mol×K	644.74	Joback Method
cpg	397.37	J/mol×K	676.99	Joback Method
cpg	406.78	J/mol×K	709.23	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=C68464368&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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