

Acetamide, 2,2,2-trifluoro-N-methyl-N-phenyl-

Other names:	Acetanilide, 2,2,2-trifluoro-N-methyl-N-Methyl-N-(trifluoroacetyl)aniline N-Methyltrifluoroacetanilide 2,2,2-Trifluoro-N-methylacetanilide 2-Trifluoromethylacetanilide
Inchi:	InChI=1S/C9H8F3NO/c1-13(8(14)9(10,11)12)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	GGDJICKTTRFKRH-UHFFFAOYSA-N
Formula:	C9H8F3NO
SMILES:	CN(C(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]:	203.16
CAS:	345-81-3

Physical Properties

Property code	Value	Unit	Source
gf	-462.42	kJ/mol	Joback Method
hf	-634.69	kJ/mol	Joback Method
hfus	19.55	kJ/mol	Joback Method
hvap	42.95	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.212		Crippen Method
mcvol	130.770	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	492.89	K	Joback Method
tc	688.82	K	Joback Method
tf	304.20	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.72	J/molxK	492.89	Joback Method
cpg	306.64	J/molxK	525.55	Joback Method
cpg	318.63	J/molxK	558.20	Joback Method
cpg	329.74	J/molxK	590.86	Joback Method

cpg	340.03	J/mol×K	623.51	Joback Method
cpg	349.53	J/mol×K	656.17	Joback Method
cpg	358.30	J/mol×K	688.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C345813&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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