

Acetamide, 2,2,2-trifluoro-N-methyl-N-(trifluoroacetyl)-

Other names:	N-Methylbis(trifluoroacetamide) 2,2,2-trifluoro-N-methyl-N-(trifluoroacetyl)acetamide
Inchi:	InChI=1S/C5H3F6NO2/c1-12(2(13)4(6,7)8)3(14)5(9,10)11/h1H3
InchiKey:	AWGBWLXGUPTXHF-UHFFFAOYSA-N
Formula:	C5H3F6NO2
SMILES:	CN(C(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]:	223.07
CAS:	685-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-1319.02	kJ/mol	Joback Method
hf	-1498.32	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	34.77	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.096		Crippen Method
mcvol	105.050	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpola	773.00		NIST Webbook
tb	423.14	K	Joback Method
tc	580.05	K	Joback Method
tf	286.82	K	Joback Method
vc	0.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.25	J/molxK	423.14	Joback Method
cpg	248.17	J/molxK	449.29	Joback Method
cpg	256.50	J/molxK	475.44	Joback Method
cpg	264.27	J/molxK	501.60	Joback Method
cpg	271.48	J/molxK	527.75	Joback Method
cpg	278.19	J/molxK	553.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C685278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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