

CF3CON(CH3)2

Other names:	Acetamide, 2,2,2-trifluoro-N,N-dimethyl- CF3CON(CH3)2
Inchi:	InChI=1S/C4H6F3NO/c1-8(2)3(9)4(5,6)7/h1-2H3
InchiKey:	WXBWKMLIVXELSF-UHFFFAOYSA-N
Formula:	C4H6F3NO
SMILES:	CN(C)C(=O)C(F)(F)F
Mol. weight [g/mol]:	141.09

Physical Properties

Property code	Value	Unit	Source
affp	849.00	kJ/mol	NIST Webbook
basg	818.00	kJ/mol	NIST Webbook
hf	-817.75	kJ/mol	Cheméo Relay (1.0)
hfus	12.56	kJ/mol	Joback Method
ie	9.72	eV	Cheméo Relay (1.0)
logp	0.637		Crippen Method
mcvol	84.080	ml/mol	McGowan Method
tb	377.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.93	J/mol×K	351.81	Joback Method
cpg	167.74	J/mol×K	378.45	Joback Method
cpg	176.08	J/mol×K	405.08	Joback Method
cpg	183.96	J/mol×K	431.72	Joback Method
cpg	191.40	J/mol×K	458.35	Joback Method
cpg	198.42	J/mol×K	484.99	Joback Method
cpg	205.03	J/mol×K	511.62	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1547871&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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