

Acetamide, 2,2,2-trifluoro-

Other names:	2,2,2-Trifluoroacetamide CF3CONH2 Trifluoroacetamide
Inchi:	InChI=1S/C2H2F3NO/c3-2(4,5)1(6)7/h(H2,6,7)
InchiKey:	NRKYWOKHZRQRJR-UHFFFAOYSA-N
Formula:	C2H2F3NO
SMILES:	NC(=O)C(F)(F)F
Mol. weight [g/mol]:	113.04
CAS:	354-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-678.10	kJ/mol	Joback Method
hf	-760.48	kJ/mol	Joback Method
hfus	9.56	kJ/mol	Joback Method
hsub	77.70 ± 1.40	kJ/mol	NIST Webbook
hvap	33.69	kJ/mol	Joback Method
ie	11.30	eV	NIST Webbook
ie	10.80	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	0.034		Crippen Method
mcvol	55.900	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
rinpol	675.00		NIST Webbook
tb	436.00 ± 1.00	K	NIST Webbook
tb	435.70	K	NIST Webbook
tc	544.65	K	Joback Method
tf	249.68	K	Joback Method
vc	0.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.85	J/mol×K	366.14	Joback Method

cpg	117.26	J/mol×K	395.89	Joback Method
cpg	122.30	J/mol×K	425.64	Joback Method
cpg	126.99	J/mol×K	455.39	Joback Method
cpg	131.35	J/mol×K	485.14	Joback Method
cpg	135.38	J/mol×K	514.89	Joback Method
cpg	139.12	J/mol×K	544.65	Joback Method
hfust	1.34	kJ/mol	388.90	NIST Webbook
hsubt	81.00	kJ/mol	308.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and thermodynamic properties of NH ₃ in choline chloride based ionic liquids:	https://www.doi.org/10.1016/j.jct.2019.01.031
Choline Based Ionic Liquids: Analogues and Their Physical Properties:	https://www.doi.org/10.1021/je100104v
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=C354381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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