N-tert-Butylacetamide

Other names:	CH3C(O)NHC(CH3)3
	N-t-Butylacetamide
	tert-Butylacetamide
	Acetamide, N-(1,1-dimethylethyl)-
Inchi:	InChI=1S/C6H13NO/c1-5(8)7-6(2,3)4/h1-4H3,(H,7,8)
InchiKey:	ACYFWRHALJTSCF-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CC(=O)NC(C)(C)C
Mol. weight [g/mol]:	115.17
CAS:	762-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-37.05	kJ/mol	Joback Method
hf	-235.03	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hsub	77.90 ± 0.40	kJ/mol	NIST Webbook
hvap	40.84	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	0.921		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	867.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1558.00		NIST Webbook
tb	437.49	K	Joback Method
tc	631.32	K	Joback Method
tf	262.39	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.96	J/mol×K	437.49	Joback Method

cpg	233.01	J/mol×K	469.80	Joback Method
cpg	244.39	J/mol×K	502.10	Joback Method
cpg	255.14	J/mol×K	534.41	Joback Method
cpg	265.29	J/mol×K	566.71	Joback Method
cpg	274.86	J/mol×K	599.02	Joback Method
cpg	283.87	J/mol×K	631.32	Joback Method
hsubt	78.30 ± 0.30	kJ/mol	286.50	NIST Webbook

Sources

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=C762845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume