N-tert-Butylmethylamine

Other names: 2-Propanamine, N,2-dimethyl-
N-Methyl-tert-butylamine
tert-butylmethylamine
Inchi: InChI=1S/C5H13N/c1-5(2,3)6-4/h6H,1-4H3
InchiKey: ZQGJEUVBUVKZKS-UHFFFAOYSA-N
Formula: C5H13N
SMILES: CNC(C)(C)C
Mol. weight [g/mol]: 87.16
CAS: 14610-37-8

Physical Properties

Property code	Value	Unit	Source
gf	83.45	kJ/mol	Joback Method
hf	-101.81	kJ/mol	Joback Method
hfus	6.39	kJ/mol	Joback Method
hvap	31.86	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.004		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	607.00		NIST Webbook
rinpol	607.00		NIST Webbook
tb	346.65 ± 1.50	K	NIST Webbook
tb	332.15 ± 4.00	K	NIST Webbook
tc	542.64	K	Joback Method
tf	201.19	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.44	J/mol×K	360.74	Joback Method
cpg	175.08	J/mol×K	391.06	Joback Method
cpg	186.14	J/mol×K	421.37	Joback Method

cpg	196.65	J/mol×K	451.69	Joback Method
cpg	206.62	J/mol×K	482.01	Joback Method
cpg	216.07	J/mol×K	512.33	Joback Method
cpg	225.03	J/mol×K	542.64	Joback Method
hvapt	32.30 ± 1.40	kJ/mol	279.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14610378&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
hvapt:	Enthalpy of vaporization at a given temperature
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