

N-tert-Butylethylamine

Inchi:	InChI=1S/C6H15N/c1-5-7-6(2,3)4/h7H,5H2,1-4H3
InchiKey:	XQOIBQBPAOVGP-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCNC(C)(C)C
Mol. weight [g/mol]:	101.19
CAS:	4432-77-3

Physical Properties

Property code	Value	Unit	Source
gf	91.87	kJ/mol	Joback Method
hf	-122.45	kJ/mol	Joback Method
hfus	8.98	kJ/mol	Joback Method
hvap	34.09	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.394		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	658.00		NIST Webbook
tb	359.15 ± 2.00	K	NIST Webbook
tc	564.84	K	Joback Method
tf	212.46	K	Joback Method
vc	0.396	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.48	J/mol×K	383.62	Joback Method
cpg	213.37	J/mol×K	413.82	Joback Method
cpg	225.63	J/mol×K	444.03	Joback Method
cpg	237.29	J/mol×K	474.23	Joback Method
cpg	248.36	J/mol×K	504.43	Joback Method
cpg	258.86	J/mol×K	534.64	Joback Method
cpg	268.84	J/mol×K	564.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C4432773&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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