N-BUTYL-TERT-BUTYLAMINE

Other names: 1-Butanamine, N-(1,1-dimethylethyl)-
N-(tert-Butyl)-1-butanamine
tert-Butyl-n-butyl-amine
N-tert-butylbutylamine
Inchi: InChI=1S/C8H19N/c1-5-6-7-9-8(2,3)4/h9H,5-7H2,1-4H3
InchiKey: VACPZDQXUAOTFR-UHFFFAOYSA-N
Formula: C8H19N
SMILES: CCCCNC(C)(C)C
Mol. weight [g/mol]: 129.25

Physical Properties

Property code	Value	Unit	Source
af	0.4063		Cheméo Relay (1.0)
hf	-166.43	kJ/mol	Cheméo Relay (1.0)
hfus	14.16	kJ/mol	Joback Method
hvap	40.72	kJ/mol	Cheméo Relay (1.0)
ie	7.66	eV	Cheméo Relay (1.0)
log10ws	-1.13		Cheméo Relay (1.0)
logp	2.175		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	839.00		NIST Webbook
rinpol	839.00		NIST Webbook
tb	403.10	K	Cheméo Relay (1.0)
tc	566.66	K	Cheméo Relay (1.0)
tf	197.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.35	J/mol×K	429.38	Joback Method
cpg	296.36	J/mol×K	459.21	Joback Method
cpg	310.65	J/mol×K	489.04	Joback Method
cpg	324.25	J/mol×K	518.88	Joback Method

cpg	337.19	J/mol×K	548.71	Joback Method
cpg	349.49	J/mol×K	578.54	Joback Method
cpg	361.18	J/mol×K	608.37	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16486741&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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