

# tert-butyl-n-octyl-amine

<b>Inchi:</b>	InChI=1S/C12H27N/c1-5-6-7-8-9-10-11-13-12(2,3)4/h13H,5-11H2,1-4H3
<b>InchiKey:</b>	UOXPORXDWKPODV-UHFFFAOYSA-N
<b>Formula:</b>	C12H27N
<b>SMILES:</b>	CCCCCCCCNC(C)(C)C
<b>Mol. weight [g/mol]:</b>	185.35
<b>CAS:</b>	38632-95-0

## Physical Properties

Property code	Value	Unit	Source
gf	142.39	kJ/mol	Joback Method
hf	-246.29	kJ/mol	Joback Method
hfus	24.52	kJ/mol	Joback Method
hvap	47.45	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.735		Crippen Method
mvol	189.920	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1233.00		NIST Webbook
tb	520.90	K	Joback Method
tc	694.12	K	Joback Method
tf	280.08	K	Joback Method
vc	0.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.14	J/mol×K	520.90	Joback Method
cpg	485.05	J/mol×K	549.77	Joback Method
cpg	502.14	J/mol×K	578.64	Joback Method
cpg	518.43	J/mol×K	607.51	Joback Method
cpg	533.95	J/mol×K	636.38	Joback Method
cpg	548.74	J/mol×K	665.25	Joback Method
cpg	562.82	J/mol×K	694.12	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C38632950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38632950&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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