

tert-butyl-n-propyl-amine

Inchi:	InChI=1S/C7H17N/c1-5-6-8-7(2,3)4/h8H,5-6H2,1-4H3
InchiKey:	LJQGARKSJMMQBX-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCNC(C)(C)C
Mol. weight [g/mol]:	115.22

Physical Properties

Property code	Value	Unit	Source
gf	100.29	kJ/mol	Joback Method
hf	-143.09	kJ/mol	Joback Method
hfus	11.57	kJ/mol	Joback Method
hvap	36.32	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.785		Crippen Method
mvol	119.470	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	744.00		NIST Webbook
rinpol	744.00		NIST Webbook
tb	406.50	K	Joback Method
tc	586.72	K	Joback Method
tf	223.73	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.82	J/mol×K	406.50	Joback Method
cpg	253.83	J/mol×K	436.54	Joback Method
cpg	267.17	J/mol×K	466.57	Joback Method
cpg	279.85	J/mol×K	496.61	Joback Method
cpg	291.91	J/mol×K	526.65	Joback Method
cpg	303.37	J/mol×K	556.69	Joback Method
cpg	314.25	J/mol×K	586.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R521914&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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