

Butanamide, N-tert.-butyl

Inchi:	InChI=1S/C8H17NO/c1-5-6-7(10)9-8(2,3)4/h5-6H2,1-4H3,(H,9,10)
InchiKey:	CABJJNMRUWQXNR-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	CCCC(=O)NC(C)(C)C
Mol. weight [g/mol]:	143.23

Physical Properties

Property code	Value	Unit	Source
gf	-20.21	kJ/mol	Joback Method
hf	-276.31	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	45.29	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.701		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinqol	1048.00		NIST Webbook
tb	483.25	K	Joback Method
tc	672.91	K	Joback Method
tf	284.93	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.10	J/mol×K	483.25	Joback Method
cpg	319.12	J/mol×K	514.86	Joback Method
cpg	332.41	J/mol×K	546.47	Joback Method
cpg	344.98	J/mol×K	578.08	Joback Method
cpg	356.87	J/mol×K	609.69	Joback Method
cpg	368.11	J/mol×K	641.30	Joback Method
cpg	378.73	J/mol×K	672.91	Joback Method

Sources

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=R50533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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