Propanamide, N-tert.-butyl-2-methyl

Inchi: InChI=1S/C8H17NO/c1-6(2)7(10)9-8(3,4)5/h6H,1-5H3,(H,9,10)
InchiKey: OEIZGTXQZLSLFL-UHFFFAOYSA-N
Formula: C8H17NO
SMILES: CC(C)C(=O)NC(C)(C)C
Mol. weight [g/mol]: 143.23

Physical Properties

Property code	Value	Unit	Source
gf	-22.65	kJ/mol	Joback Method
hf	-281.59	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	44.90	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.557		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	983.00		NIST Webbook
tb	482.81	K	Joback Method
tc	676.67	K	Joback Method
tf	269.93	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.28	J/mol×K	482.81	Joback Method
cpg	319.69	J/mol×K	515.12	Joback Method
cpg	333.32	J/mol×K	547.43	Joback Method
cpg	346.20	J/mol×K	579.74	Joback Method
cpg	358.36	J/mol×K	612.05	Joback Method
cpg	369.84	J/mol×K	644.36	Joback Method
cpg	380.66	J/mol×K	676.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R51008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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