Hexanamide, N-tert.-butyl

Inchi: InChI=1S/C10H21NO/c1-5-6-7-8-9(12)11-10(2,3)4/h5-8H2,1-4H3,(H,11,12)
InchiKey: IIDVPTZPTHTXSC-UHFFFAOYSA-N
Formula: C10H21NO
SMILES: CCCCCC(=O)NC(C)(C)C
Mol. weight [g/mol]: 171.28

Physical Properties

Property code	Value	Unit	Source
gf	-3.37	kJ/mol	Joback Method
hf	-317.59	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	49.74	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.481		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1246.00		NIST Webbook
tb	529.01	K	Joback Method
tc	714.43	K	Joback Method
tf	307.47	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.93	J/mol×K	529.01	Joback Method
cpg	412.47	J/mol×K	559.91	Joback Method
cpg	427.22	J/mol×K	590.82	Joback Method
cpg	441.20	J/mol×K	621.72	Joback Method
cpg	454.44	J/mol×K	652.62	Joback Method
cpg	466.99	J/mol×K	683.53	Joback Method
cpg	478.86	J/mol×K	714.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50743&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
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