cyclopropanecarboxamide, N-tert.-butyl

Inchi: InChI=1S/C8H15NO/c1-8(2,3)9-7(10)6-4-5-6/h6H,4-5H2,1-3H3,(H,9,10)
InchiKey: IGGMKEYOISAENY-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: CC(C)(C)NC(=O)C1CC1
Mol. weight [g/mol]: 141.21

Physical Properties

Property code	Value	Unit	Source
gf	40.54	kJ/mol	Joback Method
hf	-203.51	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	45.20	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.311		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
tb	489.99	K	Joback Method
tc	694.64	K	Joback Method
tf	302.87	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.66	J/mol×K	489.99	Joback Method
cpg	305.73	J/mol×K	524.10	Joback Method
cpg	319.79	J/mol×K	558.21	Joback Method
cpg	332.92	J/mol×K	592.32	Joback Method
cpg	345.17	J/mol×K	626.43	Joback Method
cpg	356.61	J/mol×K	660.53	Joback Method
cpg	367.29	J/mol×K	694.64	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=R50640&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