Carbodiimide, methyl tert.-butyl

Inchi: InChI=1S/C6H12N2/c1-6(2,3)8-5-7-4/h1-4H3
InchiKey: VTSXWGUXOIAASL-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CN=C=NC(C)(C)C
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
hf	34.08	kJ/mol	Joback Method
hvap	34.76	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.589		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
tb	485.92	K	Joback Method
tc	711.45	K	Joback Method

Sources

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=R511432&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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