

trans-Di-tert-butylhyponitrite

Inchi: InChI=1S/C8H18N2O2/c1-7(2,3)11-9-10-12-8(4,5)6/h1-6H3/b10-9+
InchiKey: OAPFBXRHYINFDV-MDZDMXLPSA-N
Formula: C8H18N2O2
SMILES: CC(C)(C)ON=NOC(C)(C)C
Mol. weight [g/mol]: 174.24
CAS: 82554-97-0

Physical Properties

Property code	Value	Unit	Source
chs	-5458.00 ± 7.50	kJ/mol	NIST Webbook
hf	-189.00 ± 12.00	kJ/mol	NIST Webbook
hfs	-263.00 ± 12.00	kJ/mol	NIST Webbook
hsub	74.00 ± 1.00	kJ/mol	NIST Webbook
hvap	42.30	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.899		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	570.02	K	Joback Method
tc	784.22	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C82554970&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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