trans-1,4-Di-tert-butyl-cyclohexane

Other names: trans-1,4-Bis(1,1-dimethylethyl)-cyclo
Trans-1,4-bis(1,1-dimethylethyl)cyclohexane
Inchi: InChI=1S/C14H28/c1-13(2,3)11-7-9-12(10-8-11)14(4,5)6/h11-12H,7-10H2,1-6H3/t11-,12
InchiKey: IBTCQHAOKZFUES-HAQNSBGRSA-N
Formula: C14H28
SMILES: CC(C)(C)C1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 196.37
CAS: 4789-35-9

Physical Properties

Property code	Value	Unit	Source
chs	-9108.90 ± 1.00	kJ/mol	NIST Webbook
gf	89.42	kJ/mol	Joback Method
hf	-315.81	kJ/mol	Joback Method
hfus	10.09	kJ/mol	Joback Method
hvap	44.29	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.885		Crippen Method
mcvol	197.260	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
tb	528.14	K	Joback Method
tc	739.34	K	Joback Method
tf	255.52	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.39	J/mol×K	704.14	Joback Method
cpg	594.75	J/mol×K	668.94	Joback Method
cpg	573.76	J/mol×K	633.74	Joback Method
cpg	551.35	J/mol×K	598.54	Joback Method
cpg	527.45	J/mol×K	563.34	Joback Method
cpg	501.98	J/mol×K	528.14	Joback Method

cpg	632.76	J/mol×K	739.34	Joback Method
dvisc	0.0106922	Pa×s	255.52	Joback Method
dvisc	0.0001934	Pa×s	528.14	Joback Method
dvisc	0.0002755	Pa×s	482.70	Joback Method
dvisc	0.0004225	Pa×s	437.27	Joback Method
dvisc	0.0007155	Pa×s	391.83	Joback Method
dvisc	0.0013912	Pa×s	346.39	Joback Method
dvisc	0.0033065	Pa×s	300.96	Joback Method
hfust	17.15	kJ/mol	363.20	NIST Webbook
hfust	17.15	kJ/mol	363.20	NIST Webbook

Sources

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=C4789359&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
tf: Normal melting (fusion) point
vc: Critical Volume