Cyclohexane, 1-(1,1-dimethylethyl)-4-methyl-, trans

Other names: Cyclohexane, 1-methyl-4-tert.-butyl, trans
Inchi: InChI=1S/C11H22/c1-9-5-7-10(8-6-9)11(2,3)4/h9-10H,5-8H2,1-4H3/t9-,10-
InchiKey: YCLKWKCHQLIGTA-MGCOHNPYSA-N
Formula: C11H22
SMILES: CC1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 154.29

Physical Properties

Property code	Value	Unit	Source
gf	61.32	kJ/mol	Joback Method
hf	-245.14	kJ/mol	Joback Method
hfus	9.74	kJ/mol	Joback Method
hvap	38.90	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.859		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1081.00		NIST Webbook
tb	462.73	K	Joback Method
tc	669.86	K	Joback Method
tf	219.29	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.39	J/mol×K	462.73	Joback Method
cpg	448.56	J/mol×K	635.34	Joback Method
cpg	430.80	J/mol×K	600.82	Joback Method
cpg	411.95	J/mol×K	566.30	Joback Method
cpg	391.96	J/mol×K	531.77	Joback Method
cpg	370.79	J/mol×K	497.25	Joback Method
cpg	465.26	J/mol×K	669.86	Joback Method
dvisc	0.0002587	Pa×s	462.73	Joback Method

dvisc	0.0003506	Pa×s	422.16	Joback Method
dvisc	0.0005069	Pa×s	381.58	Joback Method
dvisc	0.0007999	Pa×s	341.01	Joback Method
dvisc	0.0014280	Pa×s	300.44	Joback Method
dvisc	0.0030549	Pa×s	259.86	Joback Method
dvisc	0.0086592	Pa×s	219.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207831&Units=SI
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

Legend

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
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

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