Cyclohexanol, 4-(1,1-dimethylethyl)-, cis-

Other names: Cyclohexanol, 4-tert-butyl-, cis-
cis-4-tert-Butylcyclohexanol
4-tert-Butylcyclohexanol, (Z)-
cis-4-tert-butylcyclohexan-1-ol
Inchi: InChI=1S/C10H20O/c1-10(2,3)8-4-6-9(11)7-5-8/h8-9,11H,4-7H2,1-3H3/t8-,9+
InchiKey: CCOQPGVQAWPUPE-DTORHVGOSA-N
Formula: C10H20O
SMILES: CC(C)(C)C1CCC(O)CC1
Mol. weight [g/mol]: 156.27
CAS: 937-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-83.92	kJ/mol	Joback Method
hf	-376.73	kJ/mol	Joback Method
hfus	11.24	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
ie	9.82 ± 0.02	eV	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.584		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1225.00		NIST Webbook
tb	532.03	K	Joback Method
tc	729.03	K	Joback Method
tf	354.20 ± 3.00	K	NIST Webbook
tf	355.90 ± 3.00	K	NIST Webbook
tf	356.00 ± 4.00	K	NIST Webbook
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	372.32	J/mol×K	532.03	Joback Method
cpg	390.15	J/mol×K	564.86	Joback Method
cpg	406.99	J/mol×K	597.70	Joback Method
cpg	422.88	J/mol×K	630.53	Joback Method
cpg	437.86	J/mol×K	663.36	Joback Method
cpg	451.95	J/mol×K	696.19	Joback Method
cpg	465.20	J/mol×K	729.03	Joback Method
dvisc	0.0384558	Pa×s	268.84	Joback Method
dvisc	0.0076741	Pa×s	312.71	Joback Method
dvisc	0.0022767	Pa×s	356.57	Joback Method
dvisc	0.0008815	Pa×s	400.44	Joback Method
dvisc	0.0004116	Pa×s	444.30	Joback Method
dvisc	0.0002204	Pa×s	488.16	Joback Method
dvisc	0.0001308	Pa×s	532.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C937053&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
ie: Ionization energy
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