

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

Other names:	(E)-4-tert-Butylcyclohexanol
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-KYZUINATSA-N
Formula:	C10H20O
SMILES:	CC(C)(C)C1CCC(O)CC1
Mol. weight [g/mol]:	156.27
CAS:	21862-63-5

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	9.91 ± 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
rinsol	1245.00		NIST Webbook
tb	532.03	K	Joback Method
tc	729.03	K	Joback Method
tf	345.00 ± 14.00	K	NIST Webbook
tf	351.90 ± 3.00	K	NIST Webbook
vc	0.535	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.32	J/mol×K	532.03	Joback Method
cpg	451.95	J/mol×K	696.19	Joback Method
cpg	437.86	J/mol×K	663.36	Joback Method
cpg	422.88	J/mol×K	630.53	Joback Method
cpg	406.99	J/mol×K	597.70	Joback Method

cpg	390.15	J/molxK	564.86	Joback Method
cpg	465.20	J/molxK	729.03	Joback Method
dvisc	0.0001308	Paxs	532.03	Joback Method
dvisc	0.0002204	Paxs	488.16	Joback Method
dvisc	0.0004116	Paxs	444.30	Joback Method
dvisc	0.0008815	Paxs	400.44	Joback Method
dvisc	0.0022767	Paxs	356.57	Joback Method
dvisc	0.0076741	Paxs	312.71	Joback Method
dvisc	0.0384558	Paxs	268.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21862635&Units=SI

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
mccvol:	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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