

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

Other names:	Cyclohexanol, 4-tert-butyl- p-tert-Butylcyclohexanol 4-tert-Butylcyclohexanol 4-tert-Butylcyclohexanol,c&t USAF do-20 Padaryl 4-t-Butylcyclohexanol
Inchi:	InChI=1S/C10H20O/c1-10(2,3)8-4-6-9(11)7-5-8/h8-9,11H,4-7H2,1-3H3
InchiKey:	CCOQPGVQAWPUPE-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(C)(C)C1CCC(O)CC1
Mol. weight [g/mol]:	156.27
CAS:	98-52-2

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
log10ws	-2.80		Crippen Method
logp	2.584		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1223.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1709.00		NIST Webbook

ripol	1720.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1730.00		NIST Webbook
tb	532.03	K	Joback Method
tc	729.03	K	Joback Method
tf	268.84	K	Joback Method
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	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	Paxs	268.84	Joback Method
dvisc	0.0076741	Paxs	312.71	Joback Method
dvisc	0.0022767	Paxs	356.57	Joback Method
dvisc	0.0008815	Paxs	400.44	Joback Method
dvisc	0.0004116	Paxs	444.30	Joback Method
dvisc	0.0002204	Paxs	488.16	Joback Method
dvisc	0.0001308	Paxs	532.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.70	K	2.00	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=C98522&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/13-384-1/Cyclohexanol-4-1-1-dimethylethyl.pdf>

Generated by Cheméo on 2024-04-17 03:11:15.114328796 +0000 UTC m=+15612724.034906111.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.