

Cyclohexene, 4-(1,1-dimethylethyl)-

Other names:	Cyclohexene, 4-tert-butyl- 4-tert-Butyl-1-cyclohexene 4-tert-Butylcyclohexene 4-tertiary-Butylcyclohexene
Inchi:	InChI=1S/C10H18/c1-10(2,3)9-7-5-4-6-8-9/h4-5,9H,6-8H2,1-3H3
InchiKey:	PJTMQLHFQYFBBB-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC(C)(C)C1CC=CCC1
Mol. weight [g/mol]:	138.25
CAS:	2228-98-0

Physical Properties

Property code	Value	Unit	Source
gf	90.57	kJ/mol	Joback Method
hf	-146.38	kJ/mol	Joback Method
hfus	7.30	kJ/mol	Joback Method
hvap	37.28	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.389		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	436.00 ± 4.00	K	NIST Webbook
tc	656.08	K	Joback Method
tf	213.02	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.09	J/mol×K	443.68	Joback Method
cpg	376.03	J/mol×K	620.68	Joback Method
cpg	360.45	J/mol×K	585.28	Joback Method
cpg	343.82	J/mol×K	549.88	Joback Method
cpg	326.08	J/mol×K	514.48	Joback Method

cpg	307.19	J/mol×K	479.08	Joback Method
cpg	390.60	J/mol×K	656.08	Joback Method
dvisc	0.0002635	Paxs	443.68	Joback Method
dvisc	0.0003647	Paxs	405.24	Joback Method
dvisc	0.0005406	Paxs	366.79	Joback Method
dvisc	0.0008784	Paxs	328.35	Joback Method
dvisc	0.0016236	Paxs	289.91	Joback Method
dvisc	0.0036212	Paxs	251.46	Joback Method
dvisc	0.0107881	Paxs	213.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2228980&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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