1-Methyl-3-tert-butyl-3-cyclohexanol

Inchi: InChI=1S/C11H22O/c1-9-6-5-7-11(12,8-9)10(2,3)4/h9,12H,5-8H2,1-4H3
InchiKey: PYDPNWPNDMTDCF-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CC1CCCC(O)(C(C)(C)C)C1
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	-80.99	kJ/mol	Joback Method
hf	-382.13	kJ/mol	Joback Method
hfus	7.53	kJ/mol	Joback Method
hvap	54.43	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.974		Crippen Method
mcvol	160.860	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
tb	555.15	K	Joback Method
tc	757.01	K	Joback Method
tf	304.01	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.99	J/mol×K	555.15	Joback Method
cpg	439.20	J/mol×K	588.79	Joback Method
cpg	456.30	J/mol×K	622.44	Joback Method
cpg	472.41	J/mol×K	656.08	Joback Method
cpg	487.65	J/mol×K	689.73	Joback Method
cpg	502.11	J/mol×K	723.37	Joback Method
cpg	515.91	J/mol×K	757.01	Joback Method

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=R95840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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