

Terpinen-4-ol

Other names:	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- p-Menth-1-en-4-ol 1-Terpinen-4-ol 4-Carvomenthenol 4-Terpineol 1-Methyl-4-isopropyl-1-cyclohexen-4-ol 4-Terpinenol Terpene-4-ol Terpinene-4-ol para-Menth-1-en-4-ol 1-para-Menthen-4-ol Terpinenol-4 Terpinenolu-4 3-Cyclohexen-1-ol, 4-methyl-1-[methylethyl]- 4-methyl-1-(1-methylethyl)-3-cyclohexen-1-ol 4-methyl-1-isopropyl-3-cyclohexen-1-ol 4-Methyl-1-(methylethyl)-3-cyclohexen-1-ol Terpin-4-ol Terpine-4-ol Terpineol-4 (. +/-.)-p-Menth-1-en-4-ol NSC 147749 1-methyl-4-isopropyl-1-cyclohexen-4-ol (4-terpineol) «alpha»-Terpinen-4-ol Terpin-4-en-1-ol Terpinen-4-ol [4S-(+), 4R-(-)] 1-p-Menthen-4-ol 4-Terpeneol l-4-terpineol
Inchi:	InChI=1S/C10H18O/c1-8(2)10(11)6-4-9(3)5-7-10/h4,8,11H,5-7H2,1-3H3
InchiKey:	WRYLYDPHFGVWKC-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC1=CCC(O)(C(C)C)CC1
Mol. weight [g/mol]:	154.25
CAS:	562-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-66.65	kJ/mol	Joback Method
hf	-291.37	kJ/mol	Joback Method
hfus	8.59	kJ/mol	Joback Method
hvap	55.50	kJ/mol	NIST Webbook
log10ws	-2.89		Crippen Method
logp	2.504		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
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ripol	1624.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1600.00		NIST Webbook
tb	543.87	K	Joback Method
tc	744.05	K	Joback Method
tf	292.84	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.99	J/mol×K	543.87	Joback Method
cpg	365.13	J/mol×K	577.23	Joback Method
cpg	379.41	J/mol×K	610.60	Joback Method
cpg	392.91	J/mol×K	643.96	Joback Method
cpg	405.73	J/mol×K	677.32	Joback Method
cpg	417.96	J/mol×K	710.69	Joback Method
cpg	429.68	J/mol×K	744.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	0.80	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=C562743&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
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

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