

Cyclohexanol, 1-(1-methylethyl)

Other names:	1-(1-methylethyl)cyclohexanol
Inchi:	InChI=1S/C9H18O/c1-8(2)9(10)6-4-3-5-7-9/h8,10H,3-7H2,1-2H3
InchiKey:	ZZDMUVQELXJWCS-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CC(C)C1(O)CCCCC1
Mol. weight [g/mol]:	142.24
CAS:	3552-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-95.40	kJ/mol	Joback Method
hf	-317.04	kJ/mol	Joback Method
hfus	5.17	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.338		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	516.85	K	Joback Method
tc	716.90	K	Joback Method
tf	268.29	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.88	J/molxK	516.85	Joback Method
cpg	336.81	J/molxK	550.19	Joback Method
cpg	351.78	J/molxK	583.53	Joback Method
cpg	365.88	J/molxK	616.87	Joback Method
cpg	379.21	J/molxK	650.21	Joback Method
cpg	391.85	J/molxK	683.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C3552010&Units=SI

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

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