

Cyclohexanol, trans-2-(1-methylethyl)

Other names:	Cyclohexanol, 2-(1-methylethyl)-, trans
Inchi:	InChI=1S/C9H18O/c1-7(2)8-5-3-4-6-9(8)10/h7-10H,3-6H2,1-2H3/t8-,9+/m0/s1
InchiKey:	IXVGVVQGNQZQGD-DTWKUNHWSA-N
Formula:	C9H18O
SMILES:	CC(C)C1CCCCC1O
Mol. weight [g/mol]:	142.24

Physical Properties

Property code	Value	Unit	Source
gf	-97.62	kJ/mol	Joback Method
hf	-352.62	kJ/mol	Joback Method
hfus	12.54	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.194		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1139.00		NIST Webbook
tb	511.94	K	Joback Method
tc	704.02	K	Joback Method
tf	240.15	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.72	J/mol×K	511.94	Joback Method
cpg	338.12	J/mol×K	543.95	Joback Method
cpg	353.74	J/mol×K	575.97	Joback Method
cpg	368.59	J/mol×K	607.98	Joback Method
cpg	382.69	J/mol×K	639.99	Joback Method
cpg	396.05	J/mol×K	672.01	Joback Method
cpg	408.69	J/mol×K	704.02	Joback Method
dvisc	0.0730257	Pa×s	240.15	Joback Method

dvisc	0.0115413	Pa×s	285.45	Joback Method
dvisc	0.0030234	Pa×s	330.75	Joback Method
dvisc	0.0010937	Pa×s	376.04	Joback Method
dvisc	0.0004923	Pa×s	421.34	Joback Method
dvisc	0.0002588	Pa×s	466.64	Joback Method
dvisc	0.0001524	Pa×s	511.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R96098&Units=SI

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
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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