

2-Cyclohexen-1-ol, 3-methyl-

Other names:	1-Methyl-1-cyclohexen-3-ol 3-Methyl-2-cyclohexenol 3-Methyl-2-cyclohexen-1-ol Seudenol 3-methylcyclohex-2-en-1-ol
Inchi:	InChI=1S/C7H12O/c1-6-3-2-4-7(8)5-6/h5,7-8H,2-4H2,1H3
InchiKey:	XNDZQQSKSQTTQQD-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1=CC(O)CCC1
Mol. weight [g/mol]:	112.17
CAS:	21378-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-83.98	kJ/mol	Joback Method
hf	-239.41	kJ/mol	Joback Method
hfus	10.64	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.477		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
ripol	1552.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	475.43	K	Joback Method
tc	671.35	K	Joback Method
tf	250.13	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.33	J/mol×K	475.43	Joback Method

cpg	227.69	J/mol×K	508.08	Joback Method
cpg	239.46	J/mol×K	540.74	Joback Method
cpg	250.64	J/mol×K	573.39	Joback Method
cpg	261.25	J/mol×K	606.04	Joback Method
cpg	271.30	J/mol×K	638.70	Joback Method
cpg	280.82	J/mol×K	671.35	Joback Method
dvisc	0.0292783	Pa×s	250.13	Joback Method
dvisc	0.0072821	Pa×s	287.68	Joback Method
dvisc	0.0024975	Pa×s	325.23	Joback Method
dvisc	0.0010690	Pa×s	362.78	Joback Method
dvisc	0.0005365	Pa×s	400.33	Joback Method
dvisc	0.0003030	Pa×s	437.88	Joback Method
dvisc	0.0001873	Pa×s	475.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.20	K	0.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21378212&Units=SI
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

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
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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