

Cyclopentanol, 3-methyl-

Other names:	3-Methylcyclopentanol 3-methylcyclopentanol, mixed isomers
Inchi:	InChI=1S/C6H12O/c1-5-2-3-6(7)4-5/h5-7H,2-4H2,1H3
InchiKey:	VEALHWXMCIRWGC-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC1CCC(O)C1
Mol. weight [g/mol]:	100.16
CAS:	18729-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-108.34	kJ/mol	Joback Method
hf	-279.26	kJ/mol	Joback Method
hfus	10.39	kJ/mol	Joback Method
hvap	45.58	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.167		Crippen Method
mvol	90.410	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	836.60		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.00		NIST Webbook
tb	421.70	K	NIST Webbook
tb	424.00 ± 5.00	K	NIST Webbook
tc	626.67	K	Joback Method
tf	224.86	K	Joback Method
vc	0.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.21	J/mol×K	439.47	Joback Method
cpg	202.53	J/mol×K	470.67	Joback Method
cpg	214.29	J/mol×K	501.87	Joback Method

cpg	225.50	J/mol×K	533.07	Joback Method
cpg	236.17	J/mol×K	564.27	Joback Method
cpg	246.32	J/mol×K	595.47	Joback Method
cpg	255.97	J/mol×K	626.67	Joback Method
dvisc	0.0399340	Paxs	224.86	Joback Method
dvisc	0.0100642	Paxs	260.63	Joback Method
dvisc	0.0035374	Paxs	296.40	Joback Method
dvisc	0.0015573	Paxs	332.16	Joback Method
dvisc	0.0008042	Paxs	367.93	Joback Method
dvisc	0.0004669	Paxs	403.70	Joback Method
dvisc	0.0002961	Paxs	439.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62850e+01
Coeff. B	-4.28654e+03
Coeff. C	-5.83690e+01
Temperature range (K), min.	326.32
Temperature range (K), max.	448.99

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18729481&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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