3-Methylcyclopentanol

Other names: 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
af	0.4672		Cheméo Relay (1.0)
gf	-108.34	kJ/mol	Joback Method
hf	-262.21	kJ/mol	Cheméo Relay (1.0)
hfus	10.39	kJ/mol	Joback Method
hvap	61.23	kJ/mol	Cheméo Relay (1.0)
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.167		Crippen Method
mcvol	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	612.54	K	Cheméo Relay (1.0)
tf	237.01	K	Cheméo Relay (1.0)
vc	0.331	m3/kmol	Cheméo Relay (1.0)

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	Pa×s	224.86	Joback Method
dvisc	0.0100642	Pa×s	260.63	Joback Method
dvisc	0.0035374	Pa×s	296.40	Joback Method
dvisc	0.0015573	Pa×s	332.16	Joback Method
dvisc	0.0008042	Pa×s	367.93	Joback Method
dvisc	0.0004669	Pa×s	403.70	Joback Method
dvisc	0.0002961	Pa×s	439.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18729481&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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