

Cyclopentene, 1,2,3-trimethyl-

Other names:	1,2,3-Trimethylcyclopentene
Inchi:	InChI=1S/C8H14/c1-6-4-5-7(2)8(6)3/h6H,4-5H2,1-3H3
InchiKey:	YNEQKUWRFVQFPF-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1=C(C)C(C)CC1
Mol. weight [g/mol]:	110.20
CAS:	473-91-6

Physical Properties

Property code	Value	Unit	Source
chl	-5031.30	kJ/mol	NIST Webbook
gf	63.73	kJ/mol	Joback Method
hf	-113.13	kJ/mol	Joback Method
hfus	10.85	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.753		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	395.10 ± 0.40	K	NIST Webbook
tc	604.64	K	Joback Method
tf	216.62	K	Joback Method
vc	0.410	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.03	J/mol×K	406.84	Joback Method
cpg	219.22	J/mol×K	439.81	Joback Method
cpg	232.79	J/mol×K	472.77	Joback Method
cpg	245.74	J/mol×K	505.74	Joback Method
cpg	258.10	J/mol×K	538.71	Joback Method
cpg	269.88	J/mol×K	571.67	Joback Method
cpg	281.10	J/mol×K	604.64	Joback Method

dvisc	0.0013688	Paxs	216.62	Joback Method
dvisc	0.0008662	Paxs	248.32	Joback Method
dvisc	0.0006080	Paxs	280.03	Joback Method
dvisc	0.0004586	Paxs	311.73	Joback Method
dvisc	0.0003644	Paxs	343.43	Joback Method
dvisc	0.0003011	Paxs	375.14	Joback Method
dvisc	0.0002562	Paxs	406.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45798e+01
Coeff. B	-3.42884e+03
Coeff. C	-5.08900e+01
Temperature range (K), min.	290.80
Temperature range (K), max.	420.84

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473916&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/ci9903071
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

Legend

chl:	Standard liquid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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