

1,3-Cyclopentadiene, 1,2,3,4,5-pentamethyl-

Other names:	1,2,3,4,5-Pentamethyl-1,3-cyclopentadiene 1,2,3,4,5-Pentamethylcyclopentadiene Cyclopentadiene, 1,2,3,4,5-pentamethyl- Pentamethylcyclopentadiene
Inchi:	InChI=1S/C10H16/c1-6-7(2)9(4)10(5)8(6)3/h6H,1-5H3
InchiKey:	WQIQNKQYEUMPBM-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1=C(C)C(C)C(C)=C1C
Mol. weight [g/mol]:	136.23
CAS:	4045-44-7

Physical Properties

Property code	Value	Unit	Source
gf	91.27	kJ/mol	Joback Method
hf	-25.00	kJ/mol	NIST Webbook
hfus	16.48	kJ/mol	Joback Method
hvap	41.34	kJ/mol	Joback Method
ie	7.35	eV	NIST Webbook
ie	7.17	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	461.72	K	Joback Method
tc	660.14	K	Joback Method
tf	264.96	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.77	J/mol×K	461.72	Joback Method
cpg	290.17	J/mol×K	494.79	Joback Method
cpg	303.98	J/mol×K	527.86	Joback Method

cpg	317.21	J/molxK	560.93	Joback Method
cpg	329.87	J/molxK	594.00	Joback Method
cpg	341.98	J/molxK	627.07	Joback Method
cpg	353.54	J/molxK	660.14	Joback Method
dvisc	0.0008324	Paxs	264.96	Joback Method
dvisc	0.0006053	Paxs	297.75	Joback Method
dvisc	0.0004689	Paxs	330.55	Joback Method
dvisc	0.0003804	Paxs	363.34	Joback Method
dvisc	0.0003194	Paxs	396.13	Joback Method
dvisc	0.0002755	Paxs	428.93	Joback Method
dvisc	0.0002427	Paxs	461.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	8.68794e+00
Coeff. B	-1.71123e+03
Coeff. C	-3.32100e+01
Temperature range (K), min.	236.92
Temperature range (K), max.	540.02

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=C4045447&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/46-212-5/1-3-Cyclopentadiene-1-2-3-4-5-pentamethyl.pdf>

Generated by Cheméo on 2024-04-23 08:53:07.40420992 +0000 UTC m=+16151636.324787231.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.