

methylcyclopentadiene

Other names:	METHYL-1,3-CYCLOPENTADIENE
Inchi:	InChI=1S/C12H16/c1-7-5-11-9-3-4-10(6-9)12(11)8(7)2/h3-5,7-10,12H,6H2,1-2H3
InchiKey:	AFIMIVFSPBNZAF-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	CC1C=C2C3C=CC(C3)C2C1C
Mol. weight [g/mol]:	160.26
CAS:	26472-00-4

Physical Properties

Property code	Value	Unit	Source
gf	255.18	kJ/mol	Joback Method
hf	-15.36	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.021		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=1)		KDB
pc	2592.49	kPa	Joback Method
tb	492.41	K	Joback Method
tc	705.26	K	Joback Method
tf	280.86	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.61	J/molxK	492.41	Joback Method
cpg	355.35	J/molxK	527.89	Joback Method
cpg	373.78	J/molxK	563.36	Joback Method
cpg	390.99	J/molxK	598.84	Joback Method
cpg	407.05	J/molxK	634.31	Joback Method

cpg	422.06	J/mol×K	669.79	Joback Method
cpg	436.10	J/mol×K	705.26	Joback Method
dvisc	0.0005260	Paxs	280.86	Joback Method
dvisc	0.0006760	Paxs	316.12	Joback Method
dvisc	0.0008262	Paxs	351.38	Joback Method
dvisc	0.0009734	Paxs	386.63	Joback Method
dvisc	0.0011159	Paxs	421.89	Joback Method
dvisc	0.0012526	Paxs	457.15	Joback Method
dvisc	0.0013829	Paxs	492.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42065e+01
Coeff. B	-3.03728e+03
Coeff. C	-3.18730e+01
Temperature range (K), min.	250.09
Temperature range (K), max.	373.33

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26472004&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
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=610
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
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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