1,3-Cyclohexadiene, 3-methyl

Other names: 2-methyl-1,3-cyclohexadiene
4,5-dihydrotoluene
Inchi: InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3,5-6H,2,4H2,1H3
InchiKey: XMWINMVFKPHMJB-UHFFFAOYSA-N
Formula: C7H10
SMILES: CC1=CCCC=C1
Mol. weight [g/mol]: 94.15
CAS: 1489-57-2

Physical Properties

Property code	Value	Unit	Source
gf	90.51	kJ/mol	Joback Method
hf	-9.06	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	33.16	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	791.00		NIST Webbook
tb	387.08	K	Joback Method
tc	596.32	K	Joback Method
tf	194.31	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.21	J/mol×K	387.08	Joback Method
cpg	207.64	J/mol×K	561.45	Joback Method
cpg	197.43	J/mol×K	526.57	Joback Method
cpg	186.61	J/mol×K	491.70	Joback Method
cpg	175.15	J/mol×K	456.83	Joback Method
cpg	163.02	J/mol×K	421.95	Joback Method

cpg	217.25	J/mol×K	596.32	Joback Method
dvisc	0.0002418	Pa×s	387.08	Joback Method
dvisc	0.0003126	Pa×s	354.95	Joback Method
dvisc	0.0004254	Pa×s	322.82	Joback Method
dvisc	0.0006197	Pa×s	290.69	Joback Method
dvisc	0.0009911	Pa×s	258.57	Joback Method
dvisc	0.0018112	Pa×s	226.44	Joback Method
dvisc	0.0040402	Pa×s	194.31	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45161e+01
Coeff. B	-3.28465e+03
Coeff. C	-4.69710e+01
Temperature range (K), min.	277.82
Temperature range (K), max.	403.82

Sources

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=C1489572&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume