1,4-Cyclohexadiene, 1-methyl-

Other names: 1-Methyl-1,4-cyclohexadiene
2,5-Dihydrotoluene
1-methylcyclohexa-1,4-diene
Inchi: InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,6H,4-5H2,1H3
InchiKey: QDXQAOGNBCOEQX-UHFFFAOYSA-N
Formula: C7H10
SMILES: CC1=CCC=CC1
Mol. weight [g/mol]: 94.15
CAS: 4313-57-9

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	800.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	789.00		NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tb	387.70	K	NIST Webbook
tb	390.25 ± 0.30	K	NIST Webbook
tc	596.32	K	Joback Method
tf	201.35 ± 0.30	K	NIST Webbook
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	163.02	J/mol×K	421.95	Joback Method
cpg	175.15	J/mol×K	456.83	Joback Method
cpg	186.61	J/mol×K	491.70	Joback Method
cpg	197.43	J/mol×K	526.57	Joback Method
cpg	207.64	J/mol×K	561.45	Joback Method
cpg	217.25	J/mol×K	596.32	Joback Method
dvisc	0.0040402	Pa×s	194.31	Joback Method
dvisc	0.0018112	Pa×s	226.44	Joback Method
dvisc	0.0009911	Pa×s	258.57	Joback Method
dvisc	0.0006197	Pa×s	290.69	Joback Method
dvisc	0.0004254	Pa×s	322.82	Joback Method
dvisc	0.0003126	Pa×s	354.95	Joback Method
dvisc	0.0002418	Pa×s	387.08	Joback Method

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=C4313579&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume