1,2,3,4-tetramethylcyclohexane

Inchi: InChI=1S/C10H20/c1-7-5-6-8(2)10(4)9(7)3/h7-10H,5-6H2,1-4H3
InchiKey: OOQVBBNTNKHXSN-UHFFFAOYSA-N
Formula: C10H20
SMILES: CC1CCC(C)C(C)C1C
Mol. weight [g/mol]: 140.27
CAS: 3726-45-2

Physical Properties

Property code	Value	Unit	Source
af	0.3035		Cheméo Relay (1.0)
gf	34.64	kJ/mol	Joback Method
hf	-205.76	kJ/mol	Cheméo Relay (1.0)
hfus	16.70	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Cheméo Relay (1.0)
ie	9.16	eV	Cheméo Relay (1.0)
log10ws	-5.16		Cheméo Relay (1.0)
logp	3.325		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	444.43	K	Cheméo Relay (1.0)
tc	622.96	K	Cheméo Relay (1.0)
tf	221.18	K	Cheméo Relay (1.0)
vc	0.495	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.06	J/mol×K	433.74	Joback Method
cpg	319.44	J/mol×K	466.35	Joback Method
cpg	338.99	J/mol×K	498.96	Joback Method
cpg	357.72	J/mol×K	531.57	Joback Method
cpg	375.63	J/mol×K	564.17	Joback Method
cpg	392.74	J/mol×K	596.78	Joback Method
cpg	409.05	J/mol×K	629.39	Joback Method

dvisc	0.0014826	Pa×s	197.12	Joback Method
dvisc	0.0008678	Pa×s	236.56	Joback Method
dvisc	0.0005920	Pa×s	275.99	Joback Method
dvisc	0.0004444	Pa×s	315.43	Joback Method
dvisc	0.0003555	Pa×s	354.87	Joback Method
dvisc	0.0002974	Pa×s	394.30	Joback Method
dvisc	0.0002570	Pa×s	433.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42146e+01
Coeff. B	-3.66744e+03
Coeff. C	-6.60280e+01
Temperature range (K), min.	329.36
Temperature range (K), max.	477.95

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

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
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