Hexane, 2,3,4,5-tetramethyl-

Other names: 2,3,4,5-tetramethylhexane
Inchi: InChI=1S/C10H22/c1-7(2)9(5)10(6)8(3)4/h7-10H,1-6H3
InchiKey: BHGNYYIOYPFWKC-UHFFFAOYSA-N
Formula: C10H22
SMILES: CC(C)C(C)C(C)C(C)C
Mol. weight [g/mol]: 142.28
CAS: 52897-15-1

Physical Properties

Property code	Value	Unit	Source
gf	23.56	kJ/mol	Joback Method
hf	-270.85	kJ/mol	Joback Method
hfus	7.56	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
log10ws	-3.04		Crippen Method
logp	3.571		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	923.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	923.10		NIST Webbook
tb	428.00 ± 2.00	K	NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tc	603.70	K	Joback Method
tf	142.46	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	315.20	J/mol×K	426.44	Joback Method
cpg	332.01	J/mol×K	455.98	Joback Method
cpg	348.14	J/mol×K	485.53	Joback Method
cpg	363.61	J/mol×K	515.07	Joback Method
cpg	378.44	J/mol×K	544.61	Joback Method
cpg	392.64	J/mol×K	574.15	Joback Method
cpg	406.22	J/mol×K	603.70	Joback Method
dvisc	0.1409238	Pa×s	142.46	Joback Method
dvisc	0.0120813	Pa×s	189.79	Joback Method
dvisc	0.0027615	Pa×s	237.12	Joback Method
dvisc	0.0010315	Pa×s	284.45	Joback Method
dvisc	0.0005103	Pa×s	331.78	Joback Method
dvisc	0.0003010	Pa×s	379.11	Joback Method
dvisc	0.0001996	Pa×s	426.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40381e+01
Coeff. B	-3.46329e+03
Coeff. C	-6.16960e+01
Temperature range (K), min.	313.56
Temperature range (K), max.	458.56

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=C52897151&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