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

Other names: 2,2,4,5-Tetramethylhexane
Inchi: InChI=1S/C10H22/c1-8(2)9(3)7-10(4,5)6/h8-9H,7H2,1-6H3
InchiKey: KDRZICOOQNIJDN-UHFFFAOYSA-N
Formula: C10H22
SMILES: CC(C)C(C)CC(C)(C)C
Mol. weight [g/mol]: 142.28
CAS: 16747-42-5

Physical Properties

Property code	Value	Unit	Source
af	0.3630		KDB
gf	31.28	kJ/mol	Joback Method
hcg	6768.46	kJ/mol	KDB
hcn	6284.326	kJ/mol	KDB
hf	-269.04	kJ/mol	Joback Method
hfus	7.20	kJ/mol	Joback Method
hvap	44.40	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2220.00	kPa	KDB
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.10		NIST Webbook
tb	444.10 ± 0.30	K	NIST Webbook
tb	421.00	K	KDB
tb	421.02 ± 0.10	K	NIST Webbook
tc	598.50	K	KDB
tf	219.00	K	KDB
vc	0.544	m3/kmol	KDB
zc	0.2426900		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.88	J/mol×K	424.09	Joback Method
cpg	334.37	J/mol×K	454.16	Joback Method
cpg	351.04	J/mol×K	484.23	Joback Method
cpg	366.91	J/mol×K	514.30	Joback Method
cpg	382.02	J/mol×K	544.37	Joback Method
cpg	396.39	J/mol×K	574.44	Joback Method
cpg	410.05	J/mol×K	604.51	Joback Method
dvisc	0.0079881	Pa×s	216.41	Joback Method
dvisc	0.0446565	Pa×s	174.88	Joback Method
dvisc	0.0024872	Pa×s	257.95	Joback Method
dvisc	0.0010703	Pa×s	299.49	Joback Method
dvisc	0.0005656	Pa×s	341.02	Joback Method
dvisc	0.0003433	Pa×s	382.55	Joback Method
dvisc	0.0002298	Pa×s	424.09	Joback Method
hvapt	35.81	kJ/mol	421.00	KDB
rfi	1.41095		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39851e+01
Coeff. B	-3.38226e+03
Coeff. C	-5.99490e+01
Temperature range (K), min.	306.87
Temperature range (K), max.	449.90

Sources

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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=158
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747425&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility