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

Other names: 2,3,4,4-Tetramethylhexane
Inchi: InChI=1S/C10H22/c1-7-10(5,6)9(4)8(2)3/h8-9H,7H2,1-6H3
InchiKey: XDRDDPSGUQMOBO-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)(C)C(C)C(C)C
Mol. weight [g/mol]: 142.28
CAS: 52897-12-8

Physical Properties

Property code	Value	Unit	Source
gf	31.28	kJ/mol	Joback Method
hf	-269.04	kJ/mol	Joback Method
hfus	7.20	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	936.30		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
tb	434.75 ± 0.40	K	NIST Webbook
tb	435.95 ± 1.00	K	NIST Webbook
tc	604.51	K	Joback Method
tf	174.88	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.88	J/mol×K	424.09	Joback Method

cpg	396.39	J/mol×K	574.44	Joback Method
cpg	382.02	J/mol×K	544.37	Joback Method
cpg	366.91	J/mol×K	514.30	Joback Method
cpg	351.04	J/mol×K	484.23	Joback Method
cpg	334.37	J/mol×K	454.16	Joback Method
cpg	410.05	J/mol×K	604.51	Joback Method
dvisc	0.0002298	Pa×s	424.09	Joback Method
dvisc	0.0003433	Pa×s	382.55	Joback Method
dvisc	0.0005656	Pa×s	341.02	Joback Method
dvisc	0.0010703	Pa×s	299.49	Joback Method
dvisc	0.0024872	Pa×s	257.95	Joback Method
dvisc	0.0079881	Pa×s	216.41	Joback Method
dvisc	0.0446565	Pa×s	174.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40592e+01
Coeff. B	-3.57590e+03
Coeff. C	-5.59900e+01
Temperature range (K), min.	315.65
Temperature range (K), max.	464.77

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=C52897128&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

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