

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

Other names:	2,3,3,5-Tetramethylhexane
Inchi:	InChI=1S/C10H22/c1-8(2)7-10(5,6)9(3)4/h8-9H,7H2,1-6H3
InchiKey:	GCGFXFIPOBRMQT-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CC(C)CC(C)(C)C(C)C
Mol. weight [g/mol]:	142.28
CAS:	52897-11-7

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	45.20	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	901.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	903.30		NIST Webbook
rinpol	903.00		NIST Webbook
tb	426.00 ± 2.00	K	NIST Webbook
tc	604.51	K	Joback Method
tf	174.88	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39822e+01
Coeff. B	-3.42695e+03
Coeff. C	-6.02860e+01
Temperature range (K), min.	310.53
Temperature range (K), max.	455.52

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol161.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52897117&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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