Hexane, 2,2,3-trimethyl-

Other names: 2,2,3-Trimethylhexane
Inchi: InChI=1S/C9H20/c1-6-7-8(2)9(3,4)5/h8H,6-7H2,1-5H3
InchiKey: CBVFSZDQEHBJEQ-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCC(C)C(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 16747-25-4

Physical Properties

Property code	Value	Unit	Source
af	0.3320		KDB
ap	345.150	K	KDB
chl	-6117.22 ± 0.75	kJ/mol	NIST Webbook
gf	24.53	kJ/mol	KDB
hcg	6117.22	kJ/mol	KDB
hcn	5677.102	kJ/mol	KDB
hf	-241.40	kJ/mol	KDB
hfl	-282.70 ± 0.92	kJ/mol	NIST Webbook
hfus	8.13	kJ/mol	Joback Method
hvap	41.70	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2490.00	kPa	KDB
rinpol	821.86		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	835.50		NIST Webbook

rinpol	822.00		NIST Webbook
rinpol	823.10		NIST Webbook
rinpol	820.18		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.87		NIST Webbook
rinpol	820.26		NIST Webbook
rinpol	821.85		NIST Webbook
rinpol	822.87		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.10		NIST Webbook
rinpol	821.85		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	824.20		NIST Webbook
rinpol	823.30		NIST Webbook
rinpol	824.70		NIST Webbook
rinpol	824.80		NIST Webbook
rinpol	820.80		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	824.80		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	823.00		NIST Webbook
tb	406.55 ± 0.50	K	NIST Webbook
tb	404.85 ± 1.00	K	NIST Webbook
tb	407.40 ± 1.50	K	NIST Webbook
tb	406.80	K	KDB
tc	588.00	K	KDB
tf	153.00	K	KDB
vc	0.499	m3/kmol	KDB
zc	0.2540970		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.82	J/mol×K	579.13	Joback Method
cpg	273.89	J/mol×K	401.65	Joback Method
cpg	289.98	J/mol×K	431.23	Joback Method
cpg	305.33	J/mol×K	460.81	Joback Method
cpg	319.96	J/mol×K	490.39	Joback Method
cpg	333.90	J/mol×K	519.97	Joback Method
cpg	347.18	J/mol×K	549.55	Joback Method
dvisc	0.0002558	Pa×s	401.65	Joback Method
dvisc	0.0222427	Pa×s	178.61	Joback Method
dvisc	0.0055664	Pa×s	215.78	Joback Method
dvisc	0.0020930	Pa×s	252.96	Joback Method
dvisc	0.0010112	Pa×s	290.13	Joback Method
dvisc	0.0005763	Pa×s	327.30	Joback Method
dvisc	0.0003684	Pa×s	364.48	Joback Method
hvapt	42.20	kJ/mol	270.50	NIST Webbook
hvapt	34.77	kJ/mol	406.80	KDB
rfi	1.40820		298.15	KDB
rhol	729.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40222e+01
Coeff. B	-3.30174e+03
Coeff. C	-5.56440e+01
Temperature range (K), min.	296.04
Temperature range (K), max.	434.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	8.12646e+01
Coeff. B	-7.58830e+03
Coeff. C	-9.81514e+00
Coeff. D	5.91435e-06
Temperature range (K), min.	238.15
Temperature range (K), max.	588.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=82
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747254&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=82
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility