Hexane, 2,3,5-trimethyl-

Other names: 2,3,5-Trimethylhexane
Inchi: InChI=1S/C9H20/c1-7(2)6-9(5)8(3)4/h7-9H,6H2,1-5H3
InchiKey: ODGLTLJZCVNPBU-UHFFFAOYSA-N
Formula: C9H20
SMILES: CC(C)CC(C)C(C)C
Mol. weight [g/mol]: 128.26
CAS: 1069-53-0

Physical Properties

Property code	Value	Unit	Source
chl	-6115.88 ± 0.84	kJ/mol	NIST Webbook
gf	17.58	kJ/mol	Joback Method
hf	-242.60	kJ/mol	NIST Webbook
hfl	-284.00 ± 1.00	kJ/mol	NIST Webbook
hfus	8.50	kJ/mol	Joback Method
hvap	41.40	kJ/mol	NIST Webbook
hvap	41.40	kJ/mol	NIST Webbook
hvap	41.42	kJ/mol	NIST Webbook
hvap	41.45	kJ/mol	NIST Webbook
log10ws	-2.86		Crippen Method
logp	3.325		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	817.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	810.50		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook

rinpol	814.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	827.70	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	820.60	NIST Webbook
rinpol	814.90	NIST Webbook
rinpol	814.87	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	814.80	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	815.02	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	811.70	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	813.30	NIST Webbook
rinpol	811.40	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	812.00	NIST Webbook

rinpol	813.20		NIST Webbook
tb	403.40 ± 0.60	K	NIST Webbook
tb	403.45 ± 0.50	K	NIST Webbook
tb	403.45 ± 0.50	K	NIST Webbook
tb	402.00 ± 2.00	K	NIST Webbook
tb	404.46 ± 0.30	K	NIST Webbook
tb	404.46 ± 0.25	K	NIST Webbook
tb	404.52	K	KDB
tb	405.00 ± 0.40	K	NIST Webbook
tb	404.50	K	NIST Webbook
tb	404.52 ± 0.10	K	NIST Webbook
tc	578.35	K	Joback Method
tf	145.25 ± 0.15	K	NIST Webbook
tf	145.25 ± 0.30	K	NIST Webbook
tf	145.25	K	KDB
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.44	J/mol×K	404.00	Joback Method
cpg	287.79	J/mol×K	433.06	Joback Method
cpg	302.55	J/mol×K	462.12	Joback Method
cpg	316.72	J/mol×K	491.17	Joback Method
cpg	330.33	J/mol×K	520.23	Joback Method
cpg	343.38	J/mol×K	549.29	Joback Method
cpg	355.89	J/mol×K	578.35	Joback Method
dvisc	0.0558851	Pa×s	146.19	Joback Method
dvisc	0.0077512	Pa×s	189.16	Joback Method
dvisc	0.0022339	Pa×s	232.13	Joback Method
dvisc	0.0009496	Pa×s	275.10	Joback Method
dvisc	0.0005086	Pa×s	318.06	Joback Method
dvisc	0.0003161	Pa×s	361.03	Joback Method
dvisc	0.0002173	Pa×s	404.00	Joback Method
hvapt	34.43	kJ/mol	404.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41034e+01
Coeff. B	-3.30854e+03
Coeff. C	-5.56850e+01
Temperature range (K), min.	295.16
Temperature range (K), max.	432.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.50061e+01
Coeff. B	-8.18556e+03
Coeff. C	-1.18986e+01
Coeff. D	7.76762e-06
Temperature range (K), min.	295.15
Temperature range (K), max.	579.20

Sources

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=87
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=87
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1069530&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
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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