2-Pentene, 2,4,4-trimethyl-

Other names:	(CH3)3CCH=C(CH3)2
	2,2,4-Trimethyl-3-pentene
	2,4,4-Trimethyl-2-pentene
	2,4,4-Trimethylpent-2-ene
	DIISOBUTYLENE
Inchi:	InChI=1S/C8H16/c1-7(2)6-8(3,4)5/h6H,1-5H3
InchiKey:	LAAVYEUJEMRIGF-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC(C)=CC(C)(C)C
Mol. weight [g/mol]:	112.21
CAS:	107-40-4

Physical Properties

Property code	Value	Unit	Source
chl	-5292.30 ± 1.80	kJ/mol	NIST Webbook
gf	90.99	kJ/mol	Joback Method
hf	-109.77	kJ/mol	Joback Method
hfus	7.95	kJ/mol	Joback Method
hvap	37.40	kJ/mol	NIST Webbook
hvap	39.30	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	729.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	730.00		NIST Webbook

rinpol	726.70		NIST Webbook
rinpol	714.50		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	729.50		NIST Webbook
rinpol	729.80		NIST Webbook
rinpol	730.10		NIST Webbook
rinpol	730.50		NIST Webbook
rinpol	730.90		NIST Webbook
rinpol	731.30		NIST Webbook
rinpol	714.50		NIST Webbook
rinpol	728.20		NIST Webbook
rinpol	728.80		NIST Webbook
rinpol	729.50		NIST Webbook
rinpol	730.20		NIST Webbook
rinpol	730.90		NIST Webbook
rinpol	730.30		NIST Webbook
rinpol	729.50		NIST Webbook
rinpol	728.70		NIST Webbook
rinpol	727.80		NIST Webbook
rinpol	726.80		NIST Webbook
rinpol	725.80		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	727.50		NIST Webbook
rinpol	715.00		NIST Webbook
sl	298.70	J/mol×K	NIST Webbook
tb	378.10	K	NIST Webbook
tb	377.05 ± 0.30	K	NIST Webbook
tb	378.06 ± 0.10	K	NIST Webbook
tb	377.70 ± 0.50	K	NIST Webbook

tb	378.30 ± 0.20	K	NIST Webbook
tb	376.55 ± 0.30	K	NIST Webbook
tc	570.42	K	Joback Method
tf	166.79 ± 0.05	K	NIST Webbook
tf	166.82 ± 0.02	K	NIST Webbook
tf	166.64 ± 0.10	K	NIST Webbook
tf	166.65 ± 0.20	K	NIST Webbook
tt	166.00 ± 2.00	K	NIST Webbook
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.11	J/mol×K	383.25	Joback Method
cpg	285.30	J/mol×K	539.22	Joback Method
cpg	273.52	J/mol×K	508.03	Joback Method
cpg	261.06	J/mol×K	476.83	Joback Method
cpg	247.86	J/mol×K	445.64	Joback Method
cpg	233.89	J/mol×K	414.44	Joback Method
cpg	296.41	J/mol×K	570.42	Joback Method
cpl	233.50	J/mol×K	296.00	NIST Webbook
hfust	6.80	kJ/mol	166.00	NIST Webbook
hfust	6.78	kJ/mol	166.00	NIST Webbook
hvapt	35.20	kJ/mol	374.60	NIST Webbook
hvapt	37.20	kJ/mol	341.50	NIST Webbook
hvapt	35.70	kJ/mol	349.50	NIST Webbook
hvapt	31.90	kJ/mol	374.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38467e+01
Coeff. B	-3.04207e+03
Coeff. C	-4.83560e+01
Temperature range (K), min.	272.71
Temperature range (K), max.	404.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.52911e+01
Coeff. B	-6.92635e+03
Coeff. C	-8.93919e+00
Coeff. D	4.89798e-06
Temperature range (K), min.	166.84
Temperature range (K), max.	558.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol336.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107404&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=336

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume