1-Pentene, 3-ethyl-

Other names:	3-Ethyl-1-pentene
	3-ethylpent-1-ene
Inchi:	InChI=1S/C7H14/c1-4-7(5-2)6-3/h4,7H,1,5-6H2,2-3H3
InchiKey:	YPVPQMCSLFDIKA-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=CC(CC)CC
Mol. weight [g/mol]:	98.19
CAS:	4038-04-4

Physical Properties

Property code	Value	Unit	Source
gf	93.46	kJ/mol	Joback Method
hf	-67.66	kJ/mol	Joback Method
hfus	9.08	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	651.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	653.40		NIST Webbook
rinpol	644.70		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	656.40		NIST Webbook
rinpol	645.80		NIST Webbook

rinpol	646.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	645.00		NIST Webbook
tb	355.80	K	Joback Method
tc	526.72	K	Joback Method
tf	145.62 ± 0.04	K	NIST Webbook
tf	145.67 ± 0.03	K	NIST Webbook
tf	145.62 ± 0.01	K	NIST Webbook
tf	145.61 ± 0.04	K	NIST Webbook
tf	145.62 ± 0.01	K	NIST Webbook
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.44	J/mol×K	526.72	Joback Method
cpg	180.32	J/mol×K	355.80	Joback Method
cpg	191.94	J/mol×K	384.29	Joback Method
cpg	203.10	J/mol×K	412.77	Joback Method
cpg	213.82	J/mol×K	441.26	Joback Method
cpg	224.10	J/mol×K	469.74	Joback Method
cpg	233.97	J/mol×K	498.23	Joback Method
dvisc	0.0002256	Pa×s	355.80	Joback Method
dvisc	0.0078928	Pa×s	151.89	Joback Method
dvisc	0.0025390	Pa×s	185.88	Joback Method
dvisc	0.0011597	Pa×s	219.86	Joback Method
dvisc	0.0006534	Pa×s	253.84	Joback Method
dvisc	0.0004215	Pa×s	287.83	Joback Method
dvisc	0.0002983	Pa×s	321.82	Joback Method
hvapt	33.40	kJ/mol	346.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43088e+01

Coeff. B	-3.09988e+03
Coeff. C	-3.73720e+01
Temperature range (K), min.	258.46
Temperature range (K), max.	381.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.20557e+01
Coeff. B	-6.38455e+03
Coeff. C	-8.56668e+00
Coeff. D	6.21067e-06
Temperature range (K), min.	145.67
Temperature range (K), max.	530.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4038044&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=234

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/files/research/kdb/mol/mol234.mol

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

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

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