(Z)-3-Ethyl-4-methylpent-2-ene

Other names: 2-Pentene, 3-ethyl-4-methyl-, (Z)-
4-Methyl-3-ethyl-cis-2-pentene
Inchi: InChI=1S/C8H16/c1-5-8(6-2)7(3)4/h5,7H,6H2,1-4H3/b8-5-
InchiKey: DSTFDBMUTNIZGD-YVMONPNESA-N
Formula: C8H16
SMILES: CC=C(CC)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 42067-48-1

Physical Properties

Property code	Value	Unit	Source
gf	85.71	kJ/mol	Joback Method
hf	-106.30	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
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	2709.85	kPa	Joback Method
rinpol	767.80		NIST Webbook
rinpol	767.80		NIST Webbook
rinpol	755.80		NIST Webbook
rinpol	768.00		NIST Webbook
tb	389.20 ± 1.00	K	NIST Webbook
tb	389.00 ± 1.50	K	NIST Webbook
tc	565.46	K	Joback Method
tf	145.88	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/mol×K	386.04	Joback Method
cpg	231.45	J/mol×K	415.94	Joback Method

cpg	244.37	J/mol×K	445.85	Joback Method
cpg	256.71	J/mol×K	475.75	Joback Method
cpg	268.50	J/mol×K	505.65	Joback Method
cpg	279.75	J/mol×K	535.55	Joback Method
cpg	290.49	J/mol×K	565.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39509e+01
Coeff. B	-3.10824e+03
Coeff. C	-5.61480e+01
Temperature range (K), min.	283.64
Temperature range (K), max.	415.92

Sources

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42067481&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

Legend

cpg: Ideal gas heat capacity

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