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

Other names: 2-Pentene, 3-ethyl-4-methyl-, (E)-
4-Methyl-3-ethyl-trans-2-pentene
Inchi: InChI=1S/C8H16/c1-5-8(6-2)7(3)4/h5,7H,6H2,1-4H3/b8-5+
InchiKey: DSTFDBMUTNIZGD-VMPITWQZSA-N
Formula: C8H16
SMILES: CC=C(CC)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 42067-49-2

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	38.90	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	767.50		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	777.80		NIST Webbook
tb	387.50 ± 1.00	K	NIST Webbook
tb	387.50 ± 0.60	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	1.39340e+01
Coeff. B	-3.08041e+03
Coeff. C	-5.68300e+01
Temperature range (K), min.	282.56
Temperature range (K), max.	414.08

Sources

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
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=C42067492&Units=SI

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