3-Ethyl-3-hexene

Other names: (C2H5)2C=CHC2H5
3-Ethylhex-3-ene
3-Hexene, 3-ethyl
Inchi: InChI=1S/C8H16/c1-4-7-8(5-2)6-3/h7H,4-6H2,1-3H3
InchiKey: AUJLDZJNMXNESO-UHFFFAOYSA-N
Formula: C8H16
SMILES: CCC=C(CC)CC
Mol. weight [g/mol]: 112.21
CAS: 16789-51-8

Physical Properties

Property code	Value	Unit	Source
gf	88.15	kJ/mol	Joback Method
hf	-101.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	39.30	kJ/mol	NIST Webbook
ie	8.48 ± 0.00	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	785.90		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	785.90		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	773.00		NIST Webbook
tb	386.48	K	Joback Method
tc	561.75	K	Joback Method
tf	160.88	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	386.48	Joback Method
cpg	231.15	J/mol×K	415.69	Joback Method
cpg	243.70	J/mol×K	444.90	Joback Method
cpg	255.70	J/mol×K	474.11	Joback Method
cpg	267.18	J/mol×K	503.32	Joback Method
cpg	278.15	J/mol×K	532.54	Joback Method
cpg	288.64	J/mol×K	561.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38196e+01
Coeff. B	-3.15446e+03
Coeff. C	-5.05240e+01
Temperature range (K), min.	283.64
Temperature range (K), max.	421.28

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16789518&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

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/mol309.mol

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

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
ie:	Ionization energy
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