1-Hexene, 4-ethyl-

Other names:	4-Ethyl-1-hexene
	4-Ethylhex-1-ene
Inchi:	InChI=1S/C8H16/c1-4-7-8(5-2)6-3/h4,8H,1,5-7H2,2-3H3
InchiKey:	OPMUAJRVOWSBTP-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=CCC(CC)CC
Mol. weight [g/mol]:	112.21
CAS:	16746-85-3

Physical Properties

Property code	Value	Unit	Source
gf	101.88	kJ/mol	Joback Method
hf	-88.30	kJ/mol	Joback Method
hfus	11.67	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	2668.02	kPa	Joback Method
rinpol	755.80		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	763.50		NIST Webbook
rinpol	763.50		NIST Webbook
tb	378.68	K	Joback Method
tc	549.32	K	Joback Method
tf	163.16	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.60	J/mol×K	378.68	Joback Method
cpg	230.47	J/mol×K	407.12	Joback Method
cpg	242.84	J/mol×K	435.56	Joback Method

cpg	254.71	J/mol×K	464.00	Joback Method
cpg	266.10	J/mol×K	492.44	Joback Method
cpg	277.03	J/mol×K	520.88	Joback Method
cpg	287.50	J/mol×K	549.32	Joback Method
dvisc	0.0085772	Pa×s	163.16	Joback Method
dvisc	0.0027265	Pa×s	199.08	Joback Method
dvisc	0.0012304	Pa×s	235.00	Joback Method
dvisc	0.0006856	Pa×s	270.92	Joback Method
dvisc	0.0004381	Pa×s	306.84	Joback Method
dvisc	0.0003075	Pa×s	342.76	Joback Method
dvisc	0.0002308	Pa×s	378.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31018e+01
Coeff. B	-2.80304e+03
Coeff. C	-6.29430e+01
Temperature range (K), min.	281.69
Temperature range (K), max.	422.75

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol282.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16746853&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

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
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

Latest version available from:

https://www.chemeo.com/cid/32-449-8/1-Hexene-4-ethyl.pdf

Generated by Cheméo on 2024-10-12 07:50:55.415845425 +0000 UTC m=+3300318.052814674.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.