3-Ethylhex-1-ene

Other names: 1-Hexene, 3-ethyl-
3-Ethyl-1-hexene
Inchi: InChI=1S/C8H16/c1-4-7-8(5-2)6-3/h5,8H,2,4,6-7H2,1,3H3
InchiKey: OLGHJTHQWQKJQQ-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CC(CC)CCC
Mol. weight [g/mol]: 112.21
CAS: 3404-58-8

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	38.50	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	745.00		NIST Webbook
rinpol	744.80		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	744.80		NIST Webbook
rinpol	735.50		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	1.33341e+01
Coeff. B	-2.97754e+03
Coeff. C	-5.17290e+01
Temperature range (K), min.	279.95
Temperature range (K), max.	422.87

Sources

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=C3404588&Units=SI

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

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