(Z)-3-Ethylhex-2-ene

Other names: 2-Hexene, 3-ethyl, cis
Inchi: InChI=1S/C8H16/c1-4-7-8(5-2)6-3/h5H,4,6-7H2,1-3H3/b8-5-
InchiKey: QEMJIDSLEPYRLM-YVMONPNESA-N
Formula: C8H16
SMILES: CC=C(CC)CCC
Mol. weight [g/mol]: 112.21

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	33.44	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	793.80		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	793.80		NIST Webbook
rinpol	782.20		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

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=R293144&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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