(E)-3-Ethyl-2-methyl-1,3-hexadiene

Inchi: InChI=1S/C9H16/c1-5-7-9(6-2)8(3)4/h7H,3,5-6H2,1-2,4H3/b9-7+
InchiKey: ICVZMTIGTXBIHI-VQHVLOKHSA-N
Formula: C9H16
SMILES: C=C(C)C(=CCC)CC
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	175.86	kJ/mol	Joback Method
hf	-6.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1030.00		NIST Webbook
tb	405.92	K	Joback Method
tc	587.50	K	Joback Method
tf	156.43	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.60	J/mol×K	405.92	Joback Method
cpg	256.52	J/mol×K	436.18	Joback Method
cpg	269.78	J/mol×K	466.45	Joback Method
cpg	282.41	J/mol×K	496.71	Joback Method
cpg	294.43	J/mol×K	526.98	Joback Method
cpg	305.86	J/mol×K	557.24	Joback Method
cpg	316.74	J/mol×K	587.50	Joback Method

Sources

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=R625848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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