

(E)-2,3-Dimethylhex-3-ene

Other names:	3-Hexene, 2,3-dimethyl-, trans
Inchi:	InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h6-7H,5H2,1-4H3/b8-6+
InchiKey:	PRTXQHCLTIKAAJ-SOFGYWHQSA-N
Formula:	C8H16
SMILES:	CCC=C(C)C(C)C
Mol. weight [g/mol]:	112.21

Physical Properties

Property code	Value	Unit	Source
gf	85.71	kJ/mol	Joback Method
hf	-106.30	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	33.05	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	755.80		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	766.50		NIST Webbook
tb	386.04	K	Joback Method
tc	565.46	K	Joback Method
tf	145.88	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/molxK	386.04	Joback Method
cpg	231.45	J/molxK	415.94	Joback Method
cpg	244.37	J/molxK	445.85	Joback Method
cpg	256.71	J/molxK	475.75	Joback Method
cpg	268.50	J/molxK	505.65	Joback Method

cpg	279.75	J/mol×K	535.55	Joback Method
cpg	290.49	J/mol×K	565.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R292958&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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