Hexane, 3-methyl-4-methylene-

Other names:	2-Ethyl-3-methyl-1-pentene
	1-Pentene, 2-ethyl-3-methyl
	2-Ethyl-3-methylpent-1-ene
	3-methyl-4-methylenehexane
Inchi:	InChI=1S/C8H16/c1-5-7(3)8(4)6-2/h8H,3,5-6H2,1-2,4H3
InchiKey:	YXLCVBVDFKWWRW-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=C(CC)C(C)CC
Mol. weight [g/mol]:	112.21
CAS:	3404-67-9

Physical Properties

Property code	Value	Unit	Source
gf	93.33	kJ/mol	Joback Method
hf	-98.09	kJ/mol	Joback Method
hfus	10.36	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	2681.86	kPa	Joback Method
rinpol	748.50		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	756.90		NIST Webbook
tb	384.90 ± 2.00	K	NIST Webbook
tc	552.61	K	Joback Method
tf	149.20	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.59	J/mol×K	378.56	Joback Method

cpg	230.69	J/mol×K	407.57	Joback Method
cpg	243.26	J/mol×K	436.58	Joback Method
cpg	255.31	J/mol×K	465.59	Joback Method
cpg	266.87	J/mol×K	494.59	Joback Method
cpg	277.94	J/mol×K	523.60	Joback Method
cpg	288.55	J/mol×K	552.61	Joback Method
hvapt	36.40	kJ/mol	348.00	NIST Webbook
hvapt	36.40	kJ/mol	345.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404679&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
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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