3,4-Dimethyl-2-hexene

Other names: 2-Hexene, 3,4-dimethyl
Inchi: InChI=1S/C8H16/c1-5-7(3)8(4)6-2/h5,8H,6H2,1-4H3
InchiKey: FMNLVKMLDPGPRY-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC=C(C)C(C)CC
Mol. weight [g/mol]: 112.21
CAS: 2213-37-8

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	767.50		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	760.50		NIST Webbook
tb	388.60 ± 1.50	K	NIST Webbook
tb	388.70 ± 1.50	K	NIST Webbook
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/mol×K	386.04	Joback Method
cpg	231.45	J/mol×K	415.94	Joback Method
cpg	244.37	J/mol×K	445.85	Joback Method
cpg	256.71	J/mol×K	475.75	Joback Method

cpg	268.50	J/mol×K	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2213378&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

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