(E)-2,3-Dimethyl-3-hexene

Other names: (E)-3,4-Dimethylhex-3-ene
3-Hexene, 3,4-dimethyl-, (E)-
(E)-3-Hexene, 3,4-dimethyl
Inchi: InChI=1S/C8H16/c1-5-7(3)8(4)6-2/h5-6H2,1-4H3/b8-7+
InchiKey: XTUXVDJHGIEBAA-BQYQJAHWSA-N
Formula: C8H16
SMILES: CCC(C)=C(C)CC
Mol. weight [g/mol]: 112.21
CAS: 19550-88-0

Physical Properties

Property code	Value	Unit	Source
gf	79.60	kJ/mol	Joback Method
hf	-110.81	kJ/mol	Joback Method
hfus	14.06	kJ/mol	Joback Method
hvap	39.70	kJ/mol	NIST Webbook
ie	8.16 ± 0.00	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	776.70		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	790.60		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	760.00		NIST Webbook
tb	387.95 ± 3.00	K	NIST Webbook
tc	565.14	K	Joback Method
tf	146.92	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.01	J/mol×K	386.36	Joback Method
cpg	231.36	J/mol×K	416.16	Joback Method
cpg	244.11	J/mol×K	445.95	Joback Method
cpg	256.30	J/mol×K	475.75	Joback Method
cpg	267.94	J/mol×K	505.55	Joback Method
cpg	279.06	J/mol×K	535.34	Joback Method
cpg	289.68	J/mol×K	565.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550880&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
ie: Ionization energy
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