2,4-Hexadiene, 3,4-dimethyl-, (E,Z)-

Other names: (E),(Z)-(CH3CH=C(CH3))2
Inchi: InChI=1S/C8H14/c1-5-7(3)8(4)6-2/h5-6H,1-4H3/b7-5-,8-6+
InchiKey: PBGBMQLUDCDJQJ-CGXWXWIYSA-N
Formula: C8H14
SMILES: CC=C(C)C(C)=CC
Mol. weight [g/mol]: 110.20
CAS: 2417-88-1

Physical Properties

Property code	Value	Unit	Source
gf	159.82	kJ/mol	Joback Method
hf	3.10	kJ/mol	NIST Webbook
hfus	14.26	kJ/mol	Joback Method
hvap	33.48	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	386.65 ± 1.50	K	NIST Webbook
tc	578.76	K	Joback Method
tf	141.84	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.58	J/mol×K	390.52	Joback Method
cpg	216.76	J/mol×K	421.89	Joback Method
cpg	229.24	J/mol×K	453.27	Joback Method
cpg	241.05	J/mol×K	484.64	Joback Method
cpg	252.25	J/mol×K	516.01	Joback Method
cpg	262.84	J/mol×K	547.39	Joback Method
cpg	272.88	J/mol×K	578.76	Joback Method

Sources

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=C2417881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume