Octane, 2,6-dimethyl-, hexadehydro deriv.

Other names:	Octatriene, dimethyl- Dimethyloctatriene (4E,6E)-2,6-Dimethyl-2,4,6-octatriene 2,6-dimethyloctane, hexadehydro derivative Ocimene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7-8H,1,6H2,2-4H3/b10-8-
InchiKey:	IHPKGUQCSIINRJ-NTMALXAHSA-N
Formula:	C10H16
SMILES:	C=CC(C)=CCC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	29714-87-2

Physical Properties

Property code	Value	Unit	Source
gf	264.50	kJ/mol	Joback Method
hf	90.56	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1019.00		NIST Webbook
tb	432.96	K	Joback Method
tc	622.27	K	Joback Method
tf	162.62	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/mol×K	432.96	Joback Method
cpg	283.41	J/mol×K	464.51	Joback Method
cpg	297.33	J/mol×K	496.06	Joback Method
cpg	310.50	J/mol×K	527.62	Joback Method
cpg	322.94	J/mol×K	559.17	Joback Method
cpg	334.71	J/mol×K	590.72	Joback Method
cpg	345.84	J/mol×K	622.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29714872&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
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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