2,6-Dimethyl 4,6-octadiene (trans)

Inchi: InChI=1S/C10H18/c1-5-10(4)8-6-7-9(2)3/h5-6,8-9H,7H2,1-4H3/b8-6+,10-5+
InchiKey: NXFMFYVNTLULFW-SOYUKNQTSA-N
Formula: C10H18
SMILES: CC=C(C)C=CCC(C)C
Mol. weight [g/mol]: 138.25
CAS: 6874-39-1

Physical Properties

Property code	Value	Unit	Source
gf	182.77	kJ/mol	Joback Method
hf	-30.36	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	37.46	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1025.40		NIST Webbook
rinpol	1025.40		NIST Webbook
tb	435.96	K	Joback Method
tc	621.97	K	Joback Method
tf	163.34	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.01	J/mol×K	435.96	Joback Method
cpg	300.46	J/mol×K	466.96	Joback Method
cpg	315.13	J/mol×K	497.96	Joback Method
cpg	329.05	J/mol×K	528.97	Joback Method
cpg	342.26	J/mol×K	559.97	Joback Method
cpg	354.79	J/mol×K	590.97	Joback Method
cpg	366.69	J/mol×K	621.97	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=C6874391&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
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